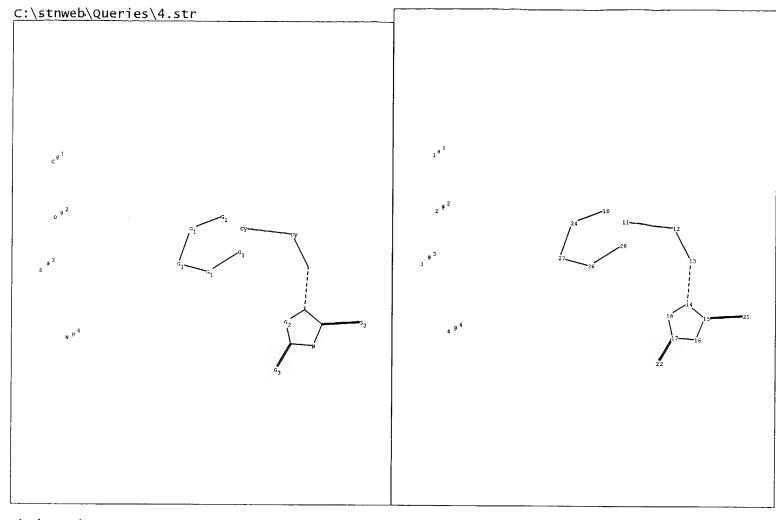


```
chain nodes :
    1 2 3 4 15 16 24
                           25
ring nodes :
    10 11 12 13 14 17
                               19 20 21
                           18
chain bonds :
    13-15
          15-16 16-17 18-24
                               20-25
ring bonds :
    10-14 11-12 12-13 13-14 17-18 17-21 18-19 19-20 20-21
exact/norm bonds :
    10-14
          11-12
                12-13 13-14 13-15 15-16 16-17 17-18 17-21 18-19 18-24 19-20 20-21
    20-25
isolated ring systems : containing 10 : 17 :
G1:[*1],[*2],[*3],[*4]
```

G2:S,N

G3:0,S

Match level: 1:CLASS 2:CLASS 3:CLASS 4:CLASS 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 24:CLASS 25:CLASS



```
chain nodes :
   1 2 3 4 12 13 21
                        22
ring nodes :
   10 11 14 15 16 17
                        18
                            24 26 27 28
chain bonds :
   11-12
         12-13 13-14 15-21
                            17-22
ring bonds :
   10-24
         14-15 14-18 15-16 16-17 17-18 24-27 26-27 26-28
exact/norm bonds :
   10-24 11-12 12-13 13-14 14-15 14-18 15-16 15-21 16-17 17-18 17-22 24-27 26-27
   26-28
isolated ring systems :
   containing 14:
```

G1:[*1],[*2],[*3],[*4]

G2:S,N

G3:0,S

Match level : 1:CLASS 2:CLASS 3:CLASS 4:CLASS 10:Atom 11:Atom 12:Atom 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 21:CLASS 22:CLASS 24:Atom 26:Atom 27:Atom 28:Atom

```
C:\stnweb\Queries\4.str
                                                      1 6 1
     c <sup>0</sup> 1
chain nodes :
    1 2 3 4 12 13 21 22
ring nodes :
    10 11 14 15 16 17
                            18
                               24 26 27 28
chain bonds:
```

```
11-12 12-13 13-14 15-21 17-22
ring bonds:
    14-15 14-18 15-16 16-17 17-18
exact/norm bonds:
    11-12 12-13 13-14 14-15 14-18 15-16 15-21 16-17 17-18 17-22
isolated ring systems:
    containing 14:

G1:[*1],[*2],[*3],[*4]

G2:s,N

G3:0,S

Match level:
    1:CLASS 2:CLASS 3:CLASS 4:CLASS 10:Atom 11:Atom 12:Atom 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 21:CLASS 22:CLASS 24:Atom 26:Atom 27:Atom 28:Atom
```

```
C:\stnweb\Queries\3.str
                                                1 e 1
chain nodes :
   1 2 3 4 12 13 21 22
ring nodes :
   10 11 14 15 16 17 18
                            24 26 27 28
chain bonds :
```

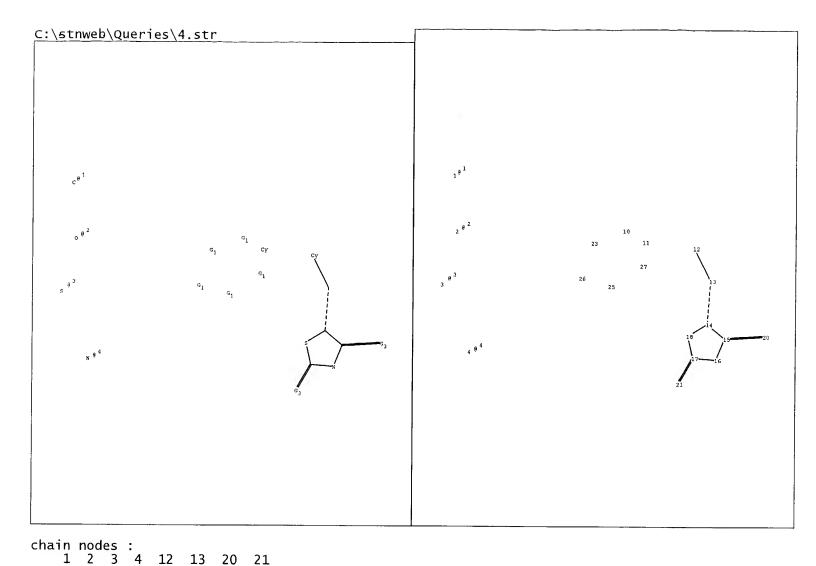
```
12-13 13-14 15-21 17-22
ring bonds:
    14-15 14-18 15-16 16-17 17-18
exact/norm bonds:
    12-13 13-14 14-15 14-18 15-16 15-21 16-17 17-18 17-22
isolated ring systems:
    containing 14:

G1:[*1],[*2],[*3],[*4]

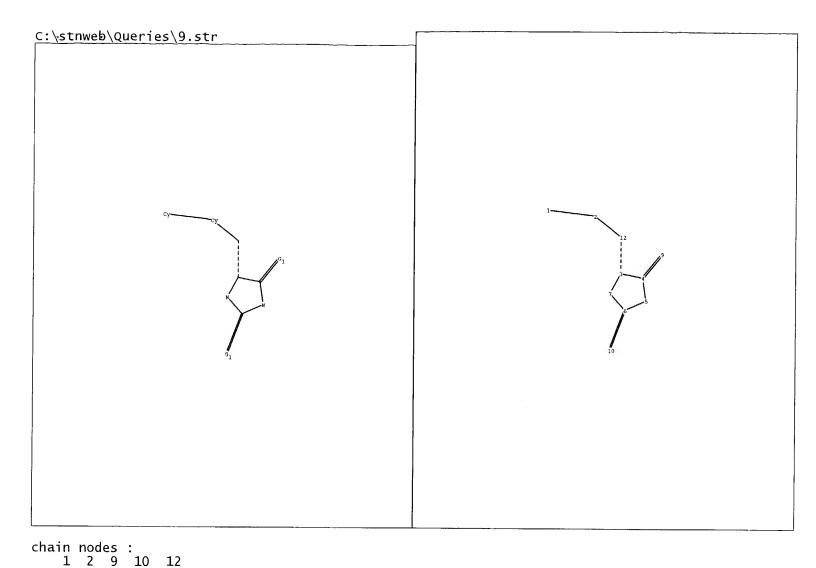
G2:S,N

G3:0,S

Match level:
    1:CLASS 2:CLASS 3:CLASS 4:CLASS 10:Atom 11:Atom 12:Atom 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 21:CLASS 24:Atom 26:Atom 27:Atom 28:Atom
```



```
ring nodes :
     10 11 14 15 16 17 18
                                   23 25 26 27
chain bonds :
    12-13 13-14 15-20 17-21
ring bonds :
    14-15 14-18 15-16 16-17
                                   17-18
exact/norm bonds:
    12-13 13-14 15-16 15-20 16-17 17-21
exact bonds :
     14-15 14-18 17-18
isolated ring systems :
    containing 14:
G1:[*1],[*2],[*3],[*4]
G3:0,S
Match level :
    1:CLASS 2:CLASS 3:CLASS 4:CLASS 10:Atom 11:Atom 12:Atom 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 20:CLASS 21:CLASS 23:Atom 25:Atom 26:Atom 27:Atom
```



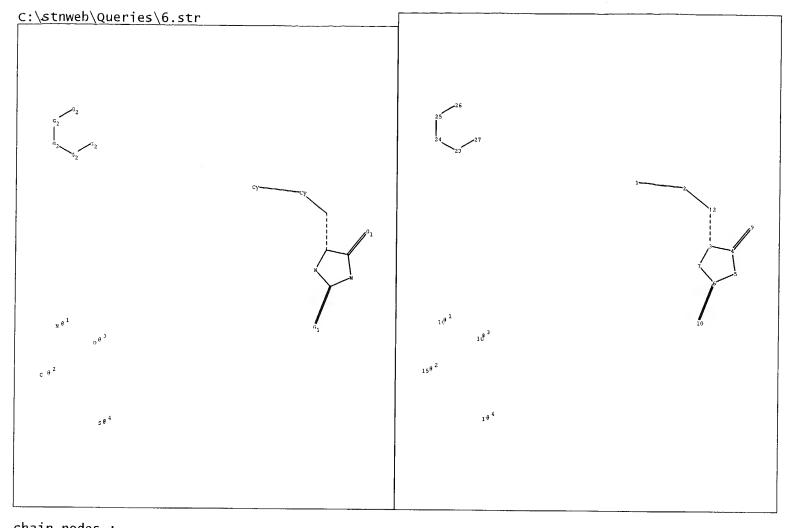
```
ring nodes:
    3    4    5    6    7
chain bonds:
    1-2   2-12   3-12   4-9   6-10
ring bonds:
    3-7   3-4   4-5   5-6   6-7
exact/norm bonds:
    1-2   2-12   3-7   3-12   4-5   4-9   5-6   6-7   6-10
exact bonds:
    3-4
isolated ring systems:
    containing 3:

G1:0,S

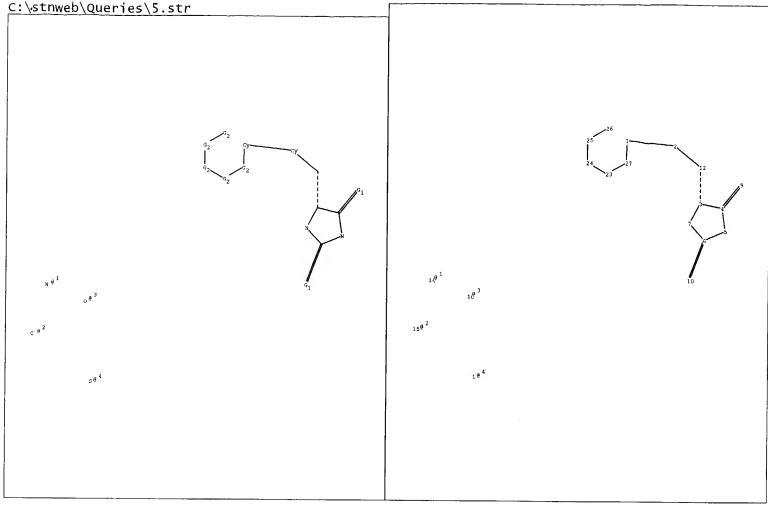
Match level:
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 9:CLASS 10:CLASS 12:CLASS
```

```
c:\stnweb\Queries\6.str
```

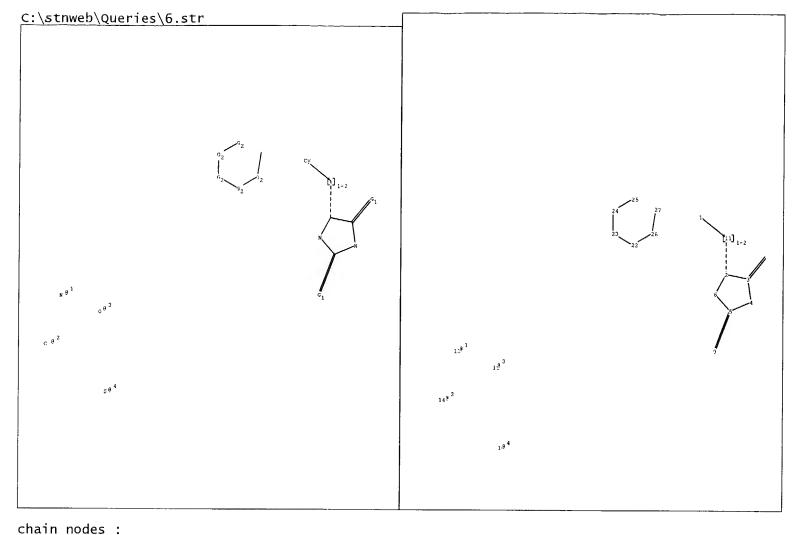
```
chain nodes :
    1 2 9 10 12 14 15 16 17 23 24 25 26 27
ring nodes:
3 4 5 6 7
chain bonds:
    1-2 2-12 3-12 4-9 6-10
ring bonds :
     3-7 3-4 4-5 5-6 6-7
exact/norm bonds :
     1-2 2-12 3-7 3-12 4-5 4-9 5-6 6-7 6-10
exact bonds :
    3-4
isolated ring systems :
    containing 3:
G1:0,S
G2:[*1],[*2],[*3],[*4]
Match level :
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 9:CLASS 10:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS
```



```
chain nodes :
    1 2 9 10 12 14 15 16 17
ring nodes : ___3 4 5 6 7 23 24 25 26 27
chain bonds:
    1-2 2-12 3-12 4-9 6-10
ring bonds :
    3-7 3-4 4-5 5-6 6-7 23-24 23-27 24-25 25-26
exact/norm bonds :
    1-2 2-12 3-7 3-12 4-5 4-9 5-6 6-7 6-10 23-24 23-27 24-25 25-26
exact bonds :
    3-4
isolated ring systems :
    containing 3:
G1:0,S
G2:[*1],[*2],[*3],[*4]
Match level :
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 9:CLASS 10:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS
```



```
chain nodes :
    2 9 10 12 14 15
                           16 17
ring nodes :
    1 3 4 5 6 7 23
                           24 25 26 27
chain bonds :
    1-2 2-12 3-12 4-9 6-10
ring bonds :
    1-27 3-7 3-4 4-5 5-6 6-7 23-24 23-27 24-25 25-26
exact/norm bonds :
    1-2 1-27 2-12 3-7 3-12 4-5 4-9 5-6 6-7 6-10 23-24 23-27 24-25 25-26
exact bonds :
    3-4
isolated ring systems:
    containing 3:
G1:0,S
G2:[*1],[*2],[*3],[*4]
Match level:
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 9:CLASS 10:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS
```



```
1 8 9 11 13 14 15 16

ring nodes:

2 3 4 5 6 22 23 24 25 26 27

chain bonds:

1-11 2-11 3-8 5-9 26-27

ring bonds:

2-6 2-3 3-4 4-5 5-6 22-23 22-26 23-24 24-25

exact/norm bonds:

1-11 2-6 2-11 3-4 3-8 4-5 5-6 5-9 22-23 22-26 23-24 24-25 26-27

exact bonds:

2-3

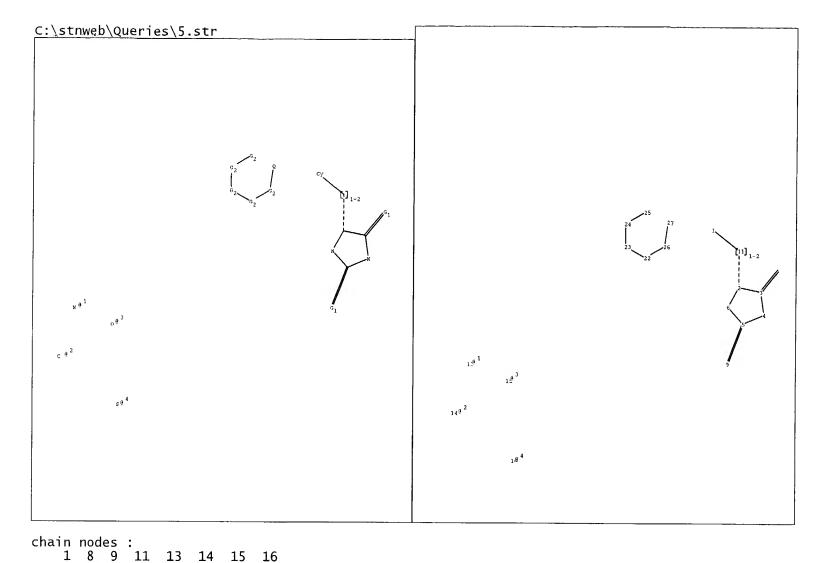
isolated ring systems:

containing 2:

G1:0,s

G2:[*1],[*2],[*3],[*4]
```

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:Atom



```
ring nodes :
    2 3 4 5 6 22 23 24 25 26 27
chain bonds :
    1-11 2-11 3-8 5-9 26-27
ring bonds :
    2-6 2-3 3-4 4-5 5-6 22-23 22-26 23-24 24-25
exact/norm bonds :
    1-11 2-6 2-11 3-4 3-8 4-5 5-6 5-9 22-23 22-26 23-24 24-25 26-27
exact bonds :
    2-3
isolated ring systems :
    containing 2:
G1:0,S
G2:[*1],[*2],[*3],[*4]
Match level:
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:Atom
```

```
C:\stnweb\Queries\6.str
```

```
1 2 4
                59
ring nodes :
                                                     22
                                                          23
                                                              24
                                                                  25
                                                                      26
                                                                          27
                                                                               28
                                                                                   29
                                                                                       30
                                                                                           31
                                     15
                                         19
                                             20
                                                 21
   6 7 8
             9
                10
                    11
                        12
                            13
                                 14
                                                              46
                                                                  47
                                                                      48
                                                                          49
                                                                               50
                                                                                   51
                                                                                       52
       33 34
                        37
                             38
                                 39
                                     40
                                         41
                                             42
                                                 43
                                                     44
                                                          45
                35
                    36
                                 68
                                     69
                                         70
                    65
                        66
                            67
           63
                64
    61 62
chain bonds :
   1-2 2-4 2-5
                  5-59
ring bonds :
                                                     12-13
                                                             13-14
                                                                    14-15
                                                                           19-20
                                                                                   19-24
               7-8 8-9
                         9-10
                                10-11
                                       10-12
                                              11-15
    6-7 6-11
                                                              29-30
                                                                     29-31
                         25-26
                                 25-30
                                        26-27
                                               27-28
                                                      28-29
                                                                            30-33
                                                                                   31-32
                                                                                           32-33
           22-23
                  23-24
    21-22
                  35-36
                         36-37
                                 37-38
                                        38-39
                                               38-40
                                                       39-42
                                                              40-41
                                                                     41-42
                                                                             43-44
                                                                                    43-48
                                                                                           44-45
    34 - 35
           34-39
                                        49-50
                  47-48
                         47-49
                                 48-52
                                               50-51
                                                       51-52
                                                              60-61
                                                                     60-65
                                                                             61 - 62
                                                                                    62-63
                                                                                           63 - 64
    45-46
           46-47
    64-65
                                        69-70
          66-67
                  66-70
                         67 - 68
                                 68 - 69
exact/norm bonds :
                   5-59
                         6-7 6-11 7-8 8-9
                                               9-10 10-11 10-12 11-15
                                                                           12-13 13-14 14-15
    1-2 2-4 2-5
                         31-32
                                 32-33
                                        38-39
                                               38-40 39-42 40-41 41-42 66-67
                                                                                    66-70 67-68
    29-30 29-31
                  30-33
    68-69 69-70
exact bonds :
                                                                                           49-50
                                                       35 - 36
                                                                            47-49
                                                                                    48-52
                  26-27
                         27-28
                                 28-29
                                        34 - 35
                                               34-39
                                                              36-37
                                                                     37-38
    25-26 25-30
    50-51
           51-52
normalized bonds :
                                                      43-48 44-45
                  20-21
                         21-22
                                 22-23
                                        23-24 43-44
                                                                    45-46 46-47 47-48
           19-24
    19-20
    60-65
           61-62 62-63
                         63-64
                                 64-65
isolated ring systems :
    containing 25 : 34 : 43 : 60 : 66 :
```

G1:0,5

G2:[*1],[*2],[*3],[*4]

G3: [*1], [*2], [*3], [*4], [*5], [*6]

Match level:

chain nodes :

12:Atom 13:Atom 14:Atom 24:Atom 25:Atom 26:Atom 34:Atom 35:Atom 36:Atom 44:Atom 45:Atom 46:Atom	15:Atom 18:CLASS	49:Atom 50:Atom	21:Atom	22:Atom 32:Atom 42:Atom 52:Atom	23:Atom
---	------------------	-----------------	---------	--	---------

```
C:\stnweb\Queries\7.str
```

```
chain nodes :
   1 2 4 5
                33
ring nodes :
    6 7 8 9 10 11 12 13 14 15 16 17 19 20 21 22 23 24 25 26 27 28 29
chain bonds :
    1-2 1-11 2-4 2-5 5-14
ring bonds :
    6-7 6-11 7-8 8-9 9-10 10-11 12-13 12-17 13-14 14-15 15-16 16-17 19-20 19-23 20-21 21-22 22-23 24-25 24-29 25-26 26-27 27-28 28-29
exact/norm bonds :
                   2-5 5-14 19-20 19-23 20-21 21-22 22-23
    1-2 1-11 2-4
normalized bonds :
    6-7 6-11 7-8 8-9 9-10 10-11 12-13 12-17 13-14 14-15 15-16 16-17 24-25 24-29 25-26 26-27 27-28 28-29
isolated ring systems :
    containing 6 : 12 : 19 : 24 :
```

G1:0,S

G4:[*1],[*2]

Match level :

1:CLASS 2:CLASS 4:CLASS 5:CLASS 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 33:CLASS 34:CLASS

```
C:\stnweb\Queries\5.str
```

```
chain nodes :
    1  2  4  5
ring nodes :
    6  7  8  9  10  11  12  13  14  15  16  17  19  20  21  22  23
chain bonds :
    1-2  1-11  2-4  2-5  5-14
ring bonds :
    6-7  6-11  7-8  8-9  9-10  10-11  12-13  12-17  13-14  14-15  15-16  16-17  19-20  19-23
    20-21  21-22  22-23
exact/norm bonds :
    1-2  1-11  2-4  2-5  5-14  19-20  19-23  20-21  21-22  22-23
normalized bonds :
    6-7  6-11  7-8  8-9  9-10  10-11  12-13  12-17  13-14  14-15  15-16  16-17
isolated ring systems :
    containing 6 : 12 : 19 :
```

G1:0,S

G4

Match level:
1:CLASS 2:CLASS 4:CLASS 5:CLASS 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 19:Atom 20:Atom 21:Atom 22:Atom
23:Atom 25:CLASS



Windows NT Printer Test Page

Congratulations!

If you can read this information, you have correctly installed your HP LaserJet 4100 PCL 6 on WS07547.

The information below describes your printer driver and port settings.

Machine Name: WS07547

Printer name: HP LaserJet 4100 PCL 6 Printer model: HP LaserJet 4100 PCL 6

Color support: Yes
Port name(s): LPT1:
Data format: RAW

Share Name: Location: Comment:

Driver name: HPBF0422.DLL Data file: HPBF0424.PMD Config file: HPBF0420.DLL

Driver version: 4.01

Environment: Windows NT x86

Monitor: HP LaserJet 5 Language Monitor

Files used by this driver:

C:\WINNT\System32\spool\DRIVERS\W32X86\2\HPBF0420.DLL (4.3.2.89)(4.3.2.89)C:\WINNT\System32\spool\DRIVERS\W32X86\2\HPBF0421.DLL C:\WINNT\System32\spool\DRIVERS\W32X86\2\HPBF0422.DLL (4.3.2.89) (4.3.2.89)C:\WINNT\System32\spool\DRIVERS\W32X86\2\HPBF0423.DLL ${\tt C:\WINNT\System32\spool\DRIVERS\W32X86\2\HPBF0424.PMD}$ C:\WINNT\System32\spool\DRIVERS\W32X86\2\HPBF0424.DLL (4.3.2.89)C:\WINNT\System32\spool\DRIVERS\W32X86\2\HPBF0424.HLP C:\WINNT\System32\spool\DRIVERS\W32X86\2\HPBF0425.DLL (4.3.2.89)C:\WINNT\System32\spool\DRIVERS\W32X86\2\HPBF0426.DLL (7.0.0.1)C:\WINNT\System32\spool\DRIVERS\W32X86\2\HPBAFD32.DLL (4.5.0)(0, 1, 0, 3) C:\WINNT\System32\spool\DRIVERS\W32X86\2\HPBFTM32.DLL C:\WINNT\System32\spool\DRIVERS\W32X86\2\HPDCMON.DLL (04.20.00)C:\WINNT\System32\spool\DRIVERS\W32X86\2\HPDCMON.DLL (04.20.00)

This is the end of the printer test page.

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			and June 2004
NEWS 5	May	12	EXTEND option available in structure searching
NEWS 6	May	12	Polymer links for the POLYLINK command completed in REGISTRY
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			SDIs in CAplus
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			CINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
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FULL ESTIMATED COST

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TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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=>

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1

STR

=> s 11

SAMPLE SEARCH INITIATED 20:08:05 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1065 TO ITERATE

93.9% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

19343 TO 23257

PROJECTED ANSWERS:

2 TO 129

L2 2 SEA SSS SAM L1

=> s 11 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 20:08:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 20966 TO ITERATE

100.0% PROCESSED 20966 ITERATIONS

24 ANSWERS

2 ANSWERS

SEARCH TIME: 00.00.01

L3 24 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST

155.84 156.05

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=> s 13

L4

9 L3

=> d 14, ibib abs fhitstr, 1-9

L4 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER:

2004:78612 HCAPLUS

DOCUMENT NUMBER:

140:136371

TITLE:

Photothermographic material

INVENTOR(S):

Nakagawa, Hajime

PATENT ASSIGNEE(S):

Japan

SOURCE:

U.S. Pat. Appl. Publ., 167 pp.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004018458	A1	20040129	US 2003-437920	20030515
JP 2003337392	A2	20031128	JP_2002-143410	20020517
JP 2004020645	A2	20040122	JP 2002-171913	20020612
JP 2004020646	A2	20040122	JP 2002-171914	20020612
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JP 2004020919	A2	20040122	JP 2002-175678	20020617
JP 2004037719	A2	20040205	JP 2002-193341	20020702
PRIORITY APPLN. INFO.:			JP 2002-143410 A	20020517
			JP 2002-171913 A	20020612
			JP 2002-171914 A	20020612
			JP 2002-172635 A	20020613
			JP 2002-174715 A	20020614
			JP 2002-175678 A	20020617
			JP 2002-193341 A	20020702

OTHER SOURCE(S): MARPAT 140:136371

AB The present invention provides a photothermog. material including a support having disposed on one surface of the support, at least one image forming layer contg. a photosensitive silver halide, a non-photosensitive org. silver salt, a reducing agent, a development accelerator and a binder, and at least one protective layer on the identical surface, wherein 50% by mass or more of the binder contained in the image forming layer is a water sol. binder, and the reducing agent is contained in the form of a solid dispersion.

IT 649569-94-8

RL: TEM (Technical or engineered material use); USES (Uses) (photothermog. material contg.)

RN 649569-94-8 HCAPLUS

CN Cyclopentanecarboxylic acid, 2-[4-[[[[3-(2,5-dihydro-5-thioxo-1H-tetrazol-1-yl)phenyl]amino]carbonyl]amino]phenyl]-5-hydroxy- (9CI) (CA INDEX NAME)

ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

Citing References Text

INVENTOR(S):

ACCESSION NUMBER: 2001:50635 HCAPLUS

DOCUMENT NUMBER: 134:115845

TITLE: Preparation of α , β -annelated butyrolactones

> as modulators of metabotropic glutamate receptors. Stolle, Andreas; Antonicek, Horst-Peter; Lensky, Stephan; Voerste, Arnd; Muller, Thomas; Baumgarten, Jorg; Von Dem Bruch, Karsten; Muller, Gerhard; Stropp,

Udo; Horvath, Ervin; De Vry, Jean-Marie-Victor;

Schreiber, Rudy

PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 215 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAT	PATENT NO. K					DATE			Α	PPLI	CATI	ON N	ο.	DATE				
WO	2001	0041	07	A	1	2001	0118		W	0 20	00-E	P610	5	2000	0630			
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		CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,	
		HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,	LS,	LT,	
		LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	PL,	PT,	RO,	RU,	
		SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	ŪĠ,	US,	UΖ,	VN,	
		YU,	ZA,	ZW,	AM,	ΑZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM					
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		DE,	DK,	ES,	FΙ,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	
		CF,	CG,	CI,	CM,	GΑ,	GN,	GW,	ML,	MR,	NE,	SN,	TD,	TG				
DE	1993	2621		A.	1	2001	0426		D	E 19	99-1	9932	621	1999	713			
PRIORITY	APP	LN.	INFO	. :]	DE 1	999-	1993:	2621	A	1999	713			
OTHER SO	URCE	(S):			MAR	PAT :	134:	1158	45									
CT																		

GT

AΒ Title compds. [I; A = CH2, CO, C(OH)R4, (CH2)aCHR5; a = 0-4; R4 = H, alkyl; R5 = Ph; R1 = H, alkyl, cycloalkyl, (benzocondensed) (substituted) heterocyclyl; R2, R3 = H, alkyl; DE = CH2COCH2, CH2CH(OH)CH2, CH2C(OH)(CH2OH)CH2, CH2C(:CR31R32)CH2, etc.; R31, R32 = H, Ph, alkyl], were prepd. for treatment of cerebral ischemia, skull/brain trauma, pain, and CNS-induced cramps (no data). Thus, N-[(3a''S*,6a''S*)-4-(5-a)]methylenehexahydrocylopenta[c]furan-1-on-6ylmethyl)phenyl]bromoacetamide

(prepn. given), Et3N, and morpholine were refluxed 20 h in PrOH to give 87% N-[(3a''S*,6a''S*)-4-(5-methylenehexahydrocylopenta[c]furan-1-on-6ylmethyl)-phenyl]-N-morpholineacetamide.

IT 321128-68-1P

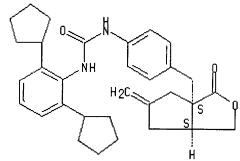
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of α, β -annelated butyrolactones as modulators of metabotropic glutamate receptors)

RN 321128-68-1 HCAPLUS

CN Urea, N-(2,6-dicyclopentylphenyl)-N'-[4-[[(3aR,6aR)-tetrahydro-5-methylene-3-oxo-1H-cyclopenta[c]furan-3a(3H)-yl]methyl]phenyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT:

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

5

Full Citing Text References

ACCESSION NUMBER: 2000:15184 HCAPLUS

DOCUMENT NUMBER: 132:64256

TITLE: Preparation of non-peptidyl inhibitors of VLA-4

dependent cell binding useful in treating

inflammatory, autoimmune and respiratory diseases

INVENTOR(S): Duplantier, Allen Jacob; Milici, Anthony John; Chupak,

Louis Stanley

PATENT ASSIGNEE(S): Pfizer Products Inc., USA

SOURCE: PCT Int. Appl., 120 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT 1	NO.		KI	ND	DATE			A.	PPLI	CATI	ON N	Ο.	DATE				
					-			-	<i>-</i>								
WO 2000	0004	77	A	1	2000	0106		W	0 19	99-I	B973		1999	0531			
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	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MD,	MG,	MK,	MN,	MW,	
	MX,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	sĸ,	SL,	TJ,	TM,	TR,	
	TT,	UA,	ŪĠ,	US,	UΖ,	VN,	YU,	ZW,	AM,	ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	TJ,	TM
RW:													CH,				
	ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	
	CI,	CM,	GA,	GN,	GW,	ML,	MR,	NE,	SN,	TD,	TG						

FS 3D CONCORD

MF C18 H20 N2 O

SR CAOLD

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS

(*File contains numerically searchable property data)

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: NORL (No role in record)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

FILE 'CAOLD' ENTERED AT 20:11:34 ON 24 JUN 2004

=> fil reg; d acc 101728-12-5; fil CAOLD

FILE 'REGISTRY' ENTERED AT 20:11:46 ON 24 JUN 2004

ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 101728-12-5 REGISTRY

CN Carbanilide, 4-bromo-4'-cyclopentylthio- (6CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H19 Br N2 S

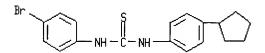
SR CAOLD

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS

(*File contains numerically searchable property data)

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: NORL (No role in record)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

FILE 'CAOLD' ENTERED AT 20:11:46 ON 24 JUN 2004

=> fil reg; d acc 102016-04-6; fil CAOLD

FILE 'REGISTRY' ENTERED AT 20:12:06 ON 24 JUN 2004

ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 102016-04-6 REGISTRY

CN Carbanilide, 4-cyclopentyl- (6CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H20 N2 O

SR CAOLD

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS

(*File contains numerically searchable property data)

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: NORL (No role in record)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

FILE 'CAOLD' ENTERED AT 20:12:07 ON 24 JUN 2004

=> fil reg; d acc 102016-04-6; fil CAOLD

FILE 'REGISTRY' ENTERED AT 20:12:25 ON 24 JUN 2004

ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 102016-04-6 REGISTRY

CN Carbanilide, 4-cyclopentyl- (6CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H20 N2 O

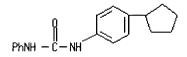
SR CAOLD

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS

(*File contains numerically searchable property data)

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: NORL (No role in record)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

FILE 'CAOLD' ENTERED AT 20:12:26 ON 24 JUN 2004

=> fil reg; d acc 102017-35-6; fil CAOLD

FILE 'REGISTRY' ENTERED AT 20:12:49 ON 24 JUN 2004

ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 102017-35-6 REGISTRY

CN Carbanilide, 4-cyclopentylthio- (6CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H20 N2 S

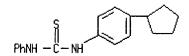
SR CAOLD

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS

(*File contains numerically searchable property data)

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: NORL (No role in record)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

FILE 'CAOLD' ENTERED AT 20:12:49 ON 24 JUN 2004

=> fil reg; d acc 102552-49-8; fil CAOLD

FILE 'REGISTRY' ENTERED AT 20:13:07 ON 24 JUN 2004

ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 102552-49-8 REGISTRY

CN Carbanilide, 4-cyclopentyl-4'-ethoxythio- (6CI) (CA INDEX NAME)

FS 3D CONCORD

MF C20 H24 N2 O S

SR CAOLD

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS

(*File contains numerically searchable property data)

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: NORL (No role in record)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

FILE 'CAOLD' ENTERED AT 20:13:08 ON 24 JUN 2004

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PRIORITY APPLN. INFO.:
                                      US 1998-91180P P 19980630
                                      WO 1999-IB973
                                                      W 19990531
                                      US 1999-338832
                                                     A3 19990623
OTHER SOURCE(S):
                MARPAT 132:64256
```

GΙ

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

The title compds. [I; A = (un) substituted aryl, heteroaryl, heterocyclyl, AB etc.; B = II-IV, etc.; E = a single bond, O, CH:CH, etc.; X = O, S, SO, SO2, etc.; Y = CO, CS, SO2, etc.; m = 0-2; n = 1-2; p = 1-2; R = CO2R5; CONO, etc.; R2, R3 = H, alkyl, alkenyl, etc.; R2R3 = (un)substituted spiro(C3-14)carbocyclic ring; R2-R4 together with the C and N atoms to which they are attached = (un) substituted heteroaryl, heterocyclyl; R5 = H, alkyl, cycloalkyl, aryl; R6 = H, alkyl, (CH2)r-cycloalkyl, etc.; r = 0-2], useful in treating or preventing an inflammatory, autoimmune or respiratory disease such as asthma, multiple sclerosis, rheumatoid arthritis, osteoarthritis, inflammatory bowel disease, psoriasis, transplant rejection, and atherosclerosis, by inhibiting cell adhesion and consequent or assocd. pathogenic processes subsequently mediated by VLA-4 (no data), were prepd. E.g., a multi-step synthesis of the title compd. V, was given. Compds. I are effective at 20 μg - 0.5 mg/kg/day.

IT 253346-52-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of non-peptidyl inhibitors of VLA-4 dependent cell binding useful in treating inflammatory, autoimmune and respiratory diseases) 253346-52-0 HCAPLUS

RN5-Oxazoleacetic acid, 2-[1-[[[4-[[[(2-cyclopentylphenyl)amino]carbonyl]ami CN no]phenyl]acetyl]amino]-3-methylbutyl]-4,5-dihydro- (9CI) (CA INDEX NAME)

2

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER: 1997:290138 HCAPLUS

DOCUMENT NUMBER:

126:263962

TITLE: 13-substituted milbemycin 5-oxime derivatives, their

preparation and their use against insects and other

pests

Patent

Sato, Kazuo; Saito, Akio; Toyama, Toshimitsu INVENTOR(S):

PATENT ASSIGNEE(S): Sankyo Co., Ltd., Japan Eur. Pat. Appl., 164 pp. SOURCE:

CODEN: EPXXDW

DOCUMENT TYPE:

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 765879	A1	19970402	EP 1996-307092	19960927
EP 765879 R: AT, BE,			, FR, GB, GR, IE, IT	, LI, LU, MC, NL,
PT, SE	•			
CA 2186650		19970330	CA 1996-2186650	19960927
NO 9604090	A	19970401	NO 1996-4090	19960927
AU 9665861	A1	19970410	AU 1996-65861	19960927
AU 707152		19990701		
ZA 9608183			ZA 1996-8183	19960927
AT 199154	E	20010215	AT 1996-307092	19960927
ES 2155172	T 3	20010501	ES 1996-307092	19960927
CZ 288178	В6	20010516	CZ 1996-2862	19960927
PT 765879	T		PT 1996-307092	19960927
CN 1153177 CN 1077110	A	19970702	CN 1996-119229	19960929
CN 1077110	В	20020102		
IL 119321	A1		IL 1996-119321	
JP 09151188	A2	19970610	JP 1996-259445	19960930
JP 3132644		20010205		
US 5861429			US 1996-723835	
RU 2128181	C1		RU 1996-120138	
HK 1003937			HK 1998-103114	19980415
GR 3035565			GR 2001-400411	
PRIORITY APPLN. INFO.	:		JP 1995-252965 A	19950929
OTHER SOURCE(S):	MA	RPAT 126:263	962	

GΙ

AB Title compds. I [R1 = Me, Et, CHMe2, CHMeEt; X = CO, CH2; R2 = alkyl; R22 = (CH2)2-5; n = 0, 1; R3 is nitro, (un)substituted amino, alkoxy, alkoxyalkoxy] having valuable acaricidal, insecticidal and anthelmintic activities were prepd. Thus, 15-hydroxy-5-oxomilbemycin A4 was acylated with 1-(4-nitrophenyl)cyclopentanecarboxylic acid, oximated, silylated, reduced to the amine, acetylated, and desilylated to give 13-[1-(4-nacetylaminophenyl)cyclopentanecarbonyloxy]-5-hydroxyiminomilbemycin A4 which gave 100% kill of cat fleas at 1 ppm in a bovine serum artificial skin prepn.

IT 188844-09-9P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

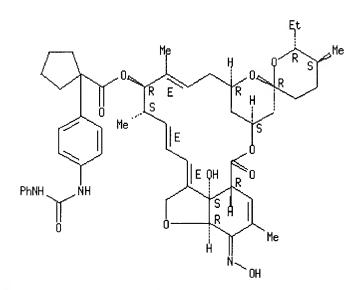
(prepn. of 13-substituted milbemycin 5-oxime derivs. as insecticides)

RN <u>188844-09-9</u> HCAPLUS

Milbemycin B, 5-demethoxy-28-deoxy-6,28-epoxy-25-ethyl-5-(hydroxyimino)-13[[[1-[4-[[(phenylamino)carbonyl]amino]phenyl]cyclopentyl]carbonyl]oxy]-,
(6R,13R,25R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as described by E or Z.



L4 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing
Text References
ACCESSION NUMBER:
DOCUMENT NUMBER:

1969:479470 HCAPLUS 71:79470

TITLE: Tuberculostatic N, N'-diarylthioureas. II AUTHOR(S): Wagner, Wolf Helmut; Winkelmann, Erhardt

CORPORATE SOURCE: Farbwerke Hoechst A.-G., Frankfurt/M.-Hoechst, Fed.

Rep. Ger.

SOURCE: Arzneimittel-Forschung (1969), 19(5), 719-30

CODEN: ARZNAD; ISSN: 0004-4172

DOCUMENT TYPE: Journal LANGUAGE: German

RNHCSNHR1 (where R = p- and (or) m-substituted phenyl; and R1 = phenylcarrying a heterocyclic or condensed heterocyclic substituent) (I) prepd. by known methods which are reviewed, were tested for tuberculostatic (I) prepd. by known methods which are reviewed, were tested for properties. (R = p-BuOC6H4 or p-iso-BuOC6H4; R1 = p-[2-(2-pyridyl)vinyl]phenyl) werethe most active, but showed long-term toxic effects in mice. In general the pyridyl residue conferred high antitubercular activity on I. be replaced by quinolyl, but replacement by other heterocycles or substitution in the pyridyl or quinolyl group caused loss of activity. Similarly the alkoxy residues in the R-substituent could be replaced by alkyl residues of the same chain length without loss of activity. The S atom is also essential for antitubercular activity. The ureas and carbamides corresponding to active thioureas showed no antitubercular activity. I (R = p-iso-BuOC6H4, p-Me2CHCH2CH2OC6H4, or p-Me2CHCH2-CH2C6H4, R1 = p-[2-(2-pyridyl)ethyl]phenyl; or <math>R =p-iso-BuOC6H4, R1 = [2-(4-pyridyl)ethyl]phenyl) had high antitubercular activity combined with lower toxicity than the corresponding pyridylvinyl derivs. I (R = p-BuOC6H4; R1 = p-Me2-NC6H4) showed antileprotic activity. IT 10400-12-1

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(antitubercular activity of)

RN <u>10400-12-1</u> HCAPLUS

CN Carbanilide, 4-cyclopentyl-4'-[2-(2-pyridyl)ethyl]thio- (7CI, 8CI) (CA INDEX NAME)

L4 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER: 1966:473373 HCAPLUS

DOCUMENT NUMBER: 65:73373 ORIGINAL REFERENCE NO.: 65:13666c-e

TITLE: α -Substituted 2-pyridinethioacetamides

INVENTOR(S): Sause, Henry W. PATENT ASSIGNEE(S): G.D. Searle and Co.

SOURCE: 10 pp.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

BE 669165 19660303 BE

PRIORITY APPLN. INFO.: US 19640903

Title products, with pharmacol. properties are prepd. as follows: H2S gas is passed through a soln. of 3 g. α -phenyl-2-pyridinoacetonitrile (I) and 1.6 g. Et3N in 120 g. pyridine for 17 hrs. at room temp. The solvent is evapd. in vacuo and the residue crystd. from hexane-iso-PrOH to give α -phenyl-2-pyridinethioacetamide (II), m. 137.5-8.0°. H2S gas is passed through a soln. of 11.4 g. α -(4-chlorophenyl)-2-pyridinoacetonitrile and 3.6 g. Et3N in 100 g. pyridine for 6 hrs. at room temp., and then left for 17 hrs. The solvent is evapd. in vacuo, and the residue crystd. from C6H6-iso-PrOH to give α -(4-chlorophenyl)-2-pyridinothioacetamide, m. 160-60.5°. A mixt. of 2.12 g. I 1.11 g. S5P5, and 8.8 g. xylene is heated with stirring for 4.5 hrs. The mixt. is cooled, dild. with benzene, and filtered. The filtrate is evapd. in vacuo, and the residue crystd. from heptane-iso-PrOH to give II, m.

vacuo, and the residue crystd. from heptane-iso-PrOH to give II, m. 135-6°. A soln. of 2.45 g. methyl α -phenyl-2-pyridinedithioacetate in 8 g. MeOH is added to 20 g. MeOH satd. with NH3.

The mixt. is left overnight, and the solvent evapd. The residue is crystd. from heptane-iso-PrOH to give II, m. 135-6°.

IT 10400-12-1, Carbanilide, 4-cyclopentyl-4'-[2-(2-pyridyl)ethyl]thio-

(prepn. of)
RN 10400-12-1 HCAPLUS

CN Carbanilide, 4-cyclopentyl-4'-[2-(2-pyridyl)ethyl]thio- (7CI, 8CI) (CA INDEX NAME)

L4 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER: 1966:473372 HCAPLUS

DOCUMENT NUMBER: 65:73372

ORIGINAL REFERENCE NO.: 65:13665h,13666a-c

TITLE: Tuberculostatic thioureas PATENT ASSIGNEE(S): Farbwerke Hoechst A.-G.

SOURCE: 12 pp.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

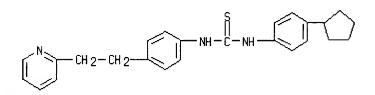
NL 6514396 19660509 NL

PRIORITY APPLN. INFO.: DE 19641106

GI For diagram(s), see printed CA Issue.

AB The title compds. (Ia) are prepd. by reaction of equimolar amts. of substituted anilines and isothiocyanates or compds. reacting as such. The reaction is optionally carried out in a 5- to 20-fold amt. of an org. solvent (such as a low-boiling alc., ether, or aromatic hydrocarbon) at the b.p. of the solvent. The products crystallize on cooling and are useful in oral and cutaneous treatment of tuberculosis and leprosy. Thus,

19.8 g. p- $(\alpha$ -pyridylethyl)aniline (I), b2 156-8°, prepd. by condensing p-nitrobenzaldehyde with α -picoline in boiling Ac20, and reducing the product with Raney Ni in EtOH, was treated in 100 ml. EtoH with 20.7 g. p-butoxyphenyl isothiocyanate; the mixt. warmed 15 min. at 75°, and kept several hrs. at room temp. The ppt. was filtered off to give 82% N-(p-butoxyphenyl)-N-[p-(α-pyridylethyl)phenyl]thiourea (II), m. 140°. II could also be prepd. by reaction of 16.5 g. p-butoxyaniline and 24 q. p- $(\alpha$ -pyridylethyl)-phenylisothiocyanate in 100 ml. EtOH, heating 15 min. at 75°, and working-up. Similarly, the following thioureas were also prepd.: N-(p-isobutoxyphenyl)-N'-[p-(\alpha-pyridylethyl)phenyl]-, m. 115°; N-(p-isoamyloxyphenyl)-N'-[p-(α-pyridylethyl)phenyl]-, m. 141°; N-(p-isobutoxyphenyl)-N'-[p-(γ-pyridylethyl)phenyl]-, m. 134°; N-(p-isoamylphenyl)- $N'-[p-(\alpha-pyridylethyl)-phenyl]-, m. 124°;$ N-(p-cyclopentylphenyl)-N'-[p-(α -pyridylethyl)phenyl]-, m. 127°; N-(p-cyclohexylphenyl)-N'-[p-(α-pyridylethyl)phenyl]-, m. 139°. IT 10400-12-1, Carbanilide, 4-cyclopentyl-4'-[2-(2-pyridyl)ethyl]thio-(prepn. of) RN 10400-12-1 HCAPLUS Carbanilide, 4-cyclopentyl-4'-[2-(2-pyridyl)ethyl]thio- (7CI, 8CI) CNINDEX NAME)



L4 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER: 1964:454881 HCAPLUS

DOCUMENT NUMBER: 61:54881
ORIGINAL REFERENCE NO.: 61:9505f-h

TITLE: Preparation of thiourea derivatives INVENTOR(S): Hilmer, Hans; Winkelmann, Ehrhardt

PATENT ASSIGNEE(S): Farbwerke Hoechst AG

SOURCE: 3 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

DE 1169943 19640514 DE 19620228

GI For diagram(s), see printed CA Issue.

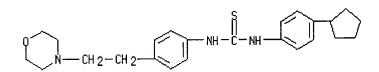
AB Thiourea compds. (I), in which R1 is a normal or branched C4~. alkyl or alkoxy group or a cyclopentylgroup and R2 is a piperidino or morpholino group, are useful against tuberculosis and leprosy. A soln. of 20.4 g. p-(2-piperidinoethyl)aniline and 20.7 g. p-iso-BuOC6H4NCS in 75 ml. EtOH was heated 20 min. at 75° and treated with an alc. HCl soln. to yield 63% I (R1 = iso-BuO, R2 = piperidino).HCl (II), m. 190°. A soln. of 16.5 g. p-iso-BuOC6H4NH2 (III) and 24.6 g. p-(2-piperidinoethyl)phenyl iso-thiocyanate in 75 ml. EtOH (20 min. at 75°) yielded also II. Similarly were prepd. I.HCl (R1, R2, m.p.,

and % yield given): BuO, piperidino, 190°, 63; iso-AmO, piperidino, 207°, 75; iso-AmO, morpholino, 241°, 63; iso-BuO, morpholino (IV), 241° 67; iso-Am, morpholino, 129°, 54; cyclopentyl, morpholino, 145°, 73. A soln. of 16.5 g. III in 100 ml. C6H6 was treated 15 min. with NH3 gas under cooling, 7.6 g. CS2 was added under stirring, and the soln. treated another 15 min. with NH3 to yield 22 g. p-iso-BuOC6H4NHCS2NH4 (V), m. 81° (decompn.). A soln. of 25.8 g. V and 20.6 g. p-(2-morpholinoethyl)aniline in 100 ml. EtOH was refluxed 2 hrs. and treated with alc. HCl soln. to yield IV.

IT 95805-72-4, Carbanilide, 4-cyclopentyl-4'-(2-morpholinoethyl)thio-(prepn. of)

RN 95805-72-4 HCAPLUS

CN Carbanilide, 4-cyclopentyl-4'-(2-morpholinoethyl)thio- (7CI) (CA INDEX NAME)



L4 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER: 1958:104298 HCAPLUS

DOCUMENT NUMBER: 52:104298

ORIGINAL REFERENCE NO.: 52:18412i,18413a-i,18414a-c

TITLE: p-Cyclopentylacetophenone and its derivatives AUTHOR(S): Hai, P. V.; Buu-Hoi, Ng. Ph.; Xuong, Ng. D.

CORPORATE SOURCE: Univ. Paris

SOURCE: Journal of Organic Chemistry (1958), 23, 39-42

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 52:104298
GI For diagram(s), see printed CA Issue.

cf. C.A. 51, 6850i. The use of the title compd. (I) prepd. from cyclopentylbenzene (II) as an intermediate for the synthesis of various aromatic and heterocyclic cyclopentyl compds., especially p-cyclopentylaniline (III) was investigated and a large no. of derivs. prepd. for evaluation of their tuberculostatic activity. Reinvestigation of the various methods proposed for the synthesis of II (cf. Cagniant, et al., C.A. 41, 6211g) showed condensation of cyclopentanol (IV) with C6H6 to be the most satisfactory. AlCl3 (17 g.) in 120 ml. C6H6 stirred vigorously with dropwise addn. of 23 g. IV and the mixt. treated with 17 q. AlCl3 and 20 q. IV, poured onto ice and the org. layer washed repeatedly with 10% NaOH, the H2O-washed org. soln. dried (CaCl2) and distd. yielded 54% II, b. 215-17°, nD20 1.5230 and 15-20% dicyclopentylbenzene, b15 178-80°, nD20 1.5427. II (14.6 g.) and 8.5 g. AcCl in 60 ml. dry CS2 stirred with portionwise addn. of 14.8 g. AlCl3 and the mixt. kept overnight at room temp., heated on a steam bath until HCl evolution stopped and decompd. with ice, the product extd. with CHCl3 and worked up as usual yielded 79% I, b15 170°, nD20 1.5509; oxime (Ia), m. 104° (alc.); semicarbazone, m. 233° (alc.). I (3.8 g.) degraded at 60-70° with aq. NaOBr (9.6 g. Br in 6.4 g. NaOH in H2O) yielded 42% p-cyclopentylbenzoic acid, m. 200° (C6H6). Similarly, 14.8 g. II, 9.2 g. EtCOCl or 10.6 g. PrCOCl, and 14.8 g. AlCl3 in 60 ml. dry CS2 gave 80% yields of p-cyclopentylpropiophenone, b17 182°, nD19 1.5439, and p-cyclopentylbutyrophenone, b27

204-6°, nD19 1.5437. Equimolar amts. of I and the appropriate aldehyde shaken in warm alc. with a few drops of 20% aq. NaOH and the ppt. recrystd. (alc.) gave a series of chalcones, p-C5H9C6H4COCH:CHR (R and m.p. given): 2-furyl, 99°; 2-thenyl, 105°; 1-naphthyl, 98°; 3-ClC6H4, 106°; 3-MeOC6H4, 84°. Ia(20.3 g.) in 100 ml. dry Et20 stirred with portionwise addn. of 31 g. finely powd. PC15 and the Et2O evapd., the residue decompd. with ice and the ppt. recrystd. (alc.) gave 16 g. p-C5H9C6H4NHAc, m. 136°, hydrolyzed (20.3 g.) by refluxing 2 hrs. with 30 ml. HCl in 100 ml. alc. and working up to yield 12 q. III, b22 165-7°, nD19 1.5710. III (3.3 g.) and 4 g. (AcCH2)2 refluxed 30 min. and distd. in vacuo gave 3 g. 1-p-cyclopentyl-2,5dimethylpyrrole, b25 207° m. 42° (MeOH). III (0.8 g.), 1.2 g. 2,3-dichloro-1,4-naphthoquinone, and 1.2 g. NaOAc refluxed 1 hr. in alc. and the ppt. formed on cooling recrystd. (alc.-C6H6) gave violet needles of 2-chloro-3-(p-cyclopentylanilino)-1,4-naphthoquinone, m. 158°. Similarly 1 g. III, 0.9 g. chloranil, and 2 g. NaOAc refluxed 1 hr. in alc. gave brown leaflets of 3,6-bis(pcyclopentylanilino)-2,5-dichloro-1,4-benzoquinone, m. 309° (PhMe). Tetrachlorophthalic anhydride (1 g.) in 15 ml. boiling AcOH treated dropwise with 0.6 g. III and the mixt. refluxed a few min. cooled and the solid crystd. (AcOH) gave N-(p-cyclopentylphenyl)tetrachlorophthalimide, m. 242°. In view of the pronounced in vitro tuberculostatic activity of various N-arylglycines (B. H., et al., C.A. 52, 3011d). (3.2 q.), 2 q. ClCH2CO2H, and 6 g. NaOAc were heated in H2O 1 hr. on a steam bath and the cooled soln. dild. with H2O. filtered and the ppt. taken up in 10% aq. (NH4)2CO3, the filtered soln. acidified with AcOH and the ppt. crystd. H2O to yield 50% p-C5H9C6H4NHCH2CO2H, m. 199°. III (6.4 g.), 8 g. BrCH2CO2Et, and 15 g. NaOAc heated 3 hrs. on a steam bath and dild. with 50 ml. H2O, extd. with CHCl3 and the washed and dried ext. evapd., the residue fractionated and the ester (77%, b15 219-21°) crystd. (petr. ether) gave p-C5H9C6H4NHCH2CO2Et (V), m. 42°. V (2.5 g.) and 1.5 g. 98% N2H4.H2O refluxed 2 hrs. in 20 ml. alc. and cooled yielded 98% p-C5H9C6H4NHCH2CONHNH2, m. 153°. The condensation of III with various aryl isothiocyanates in equimolar amts. by heating 30 min. at 50-60° in alc. and crystn. (alc.) of the product gave a series of bitter tasting substituted pcyclopentylthiocarbanilides, p-C5H9C6H4NHCSNHR (R and m.p. given): Ph, 142°; 4-FC6H4, 177°; 4-ClC6H4, 208°; 4-BrC6H4, 215°; 4-Me-C6H4, 158°; 2,4-Me2C6H3, 145°; 4-EtC6H4, 130°; 4-EtOC6H4, 167°; 4-Me2CH(CH2)2OC6H4, 128°; 2-PhC6H4, 187°; 4-C5H9C6H4, 203°. These compds. with the exception of the 4-BrC6H4 and 2-PhC6H4 derivs. showed considerable in vitro tuberculostatic activity against Mycobacterium tuberculosis (H37 RvD) at a concn. of 10 γ/ml . Dubos culture medium. similarly synthesized substituted p-cyclopentylcarbanilides, p-C5H9C6H4NHCONHR (R and m.p. given): Ph, 195°; p-ClC6H4, 229°; 2-PhC6H4, 169°; 2-Cl0H7, 220°, were found inactive against M. tuberculosis. Fischer indolization of I phenylhydrazone readily afforded 2-(p-cyclopentylphenyl)indole (VI). I (3 q.) and 2 q. PhNHNH2 heated a few min. at 140-50° with loss of H2O and the crude phenylhydrazone heated 15 min. at 185-95° with 7 g. finely powd., fused ZnCl2, the cooled mixt. treated with AcOH and extd. with C6H6, the H2O-washed ext. dried (Na2SO4) and evapd., the residue distd. in vacuo and the fraction, b13 270-2° recrystd. (C6H6-alc.) yielded 70% VI, m. 236°; picrate, deep-violet. Isatin (1 mole) and 1 mole I (and its higher homologs) gently refluxed 72 hrs. on a steam bath with 20% alc. KOH (3 moles KOH) and the soln. dild. with H2O, the neutral impurities extd. with Et2O and the aq. layer acidified with AcOH, the pptd. cinchonic acid washed with H2O and recrystd. (alc.) gave 30% to 80-5% yields of substituted 2-(p-cyclopentylphenyl)cinchonic acids (VII)

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(*File contains numerically searchable property data)

DT.CA CAplus document type: Journal; Patent

RL.P Roles from patents: NORL (No role in record)

RL.NP Roles from non-patents: BIOL (Biological study); USES (Uses)

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FS 3D CONCORD

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LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS

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DT.CA CAplus document type: Patent

RL.P Roles from patents: NORL (No role in record)

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RN 1536-16-9 REGISTRY

CN Carbanilide, 4-cyclopentyl-4'-fluorothio- (6CI, 8CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H19 F N2 S

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS

(*File contains numerically searchable property data)

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: NORL (No role in record)

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ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 1536-16-9 REGISTRY

CN Carbanilide, 4-cyclopentyl-4'-fluorothio- (6CI, 8CI) (CA INDEX NAME)

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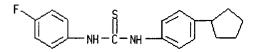
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LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS

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DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: NORL (No role in record)



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ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 101728-12-5 REGISTRY

CN Carbanilide, 4-bromo-4'-cyclopentylthio- (6CI) (CA INDEX NAME)

FS 3D CONCORD

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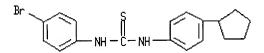
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RN 102004-95-5 REGISTRY

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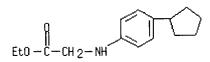
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LC STN Files: BEILSTEIN*, CAOLD

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1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 113649-89-1 REGISTRY

CN Carbanilide, 4'-cyclopentyl-2-phenylthio- (6CI) (CA INDEX NAME)

FS 3D CONCORD

MF C24 H24 N2 S

SR CAOLD

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS

(*File contains numerically searchable property data)

DT.CA Caplus document type: Journal

RL.NP Roles from non-patents: NORL (No role in record)

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1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 102747-60-4 REGISTRY

CN Carbanilide, 4'-cyclopentyl-2-phenyl- (6CI) (CA INDEX NAME)

FS 3D CONCORD

MF C24 H24 N2 O

SR CAOLD

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS

(*File contains numerically searchable property data)

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: NORL (No role in record)

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- 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 102458-17-3 REGISTRY

CN Carbanilide, 4'-cyclopentyl-2,4-dimethylthio- (6CI) (CA INDEX NAME)

FS 3D CONCORD

MF C20 H24 N2 S

SR CAOLD

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS

(*File contains numerically searchable property data)

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: NORL (No role in record)

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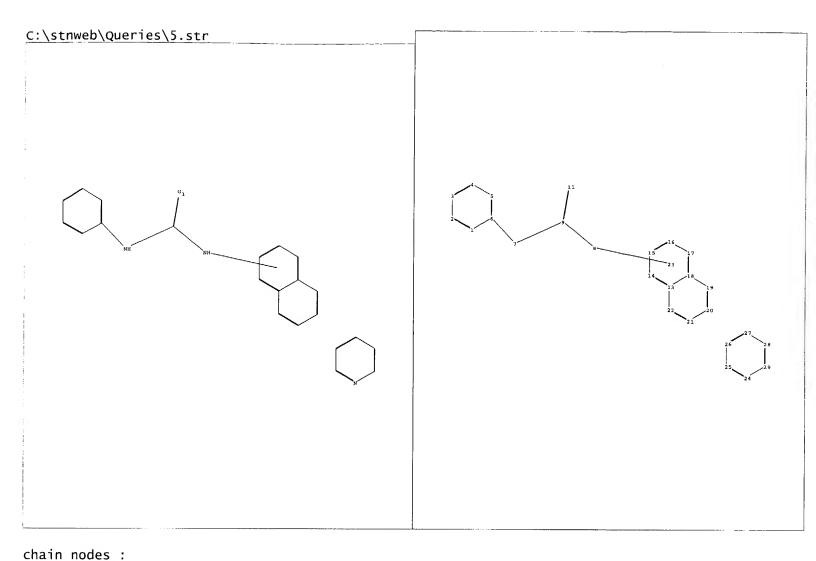
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ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 102016-04-6 REGISTRY

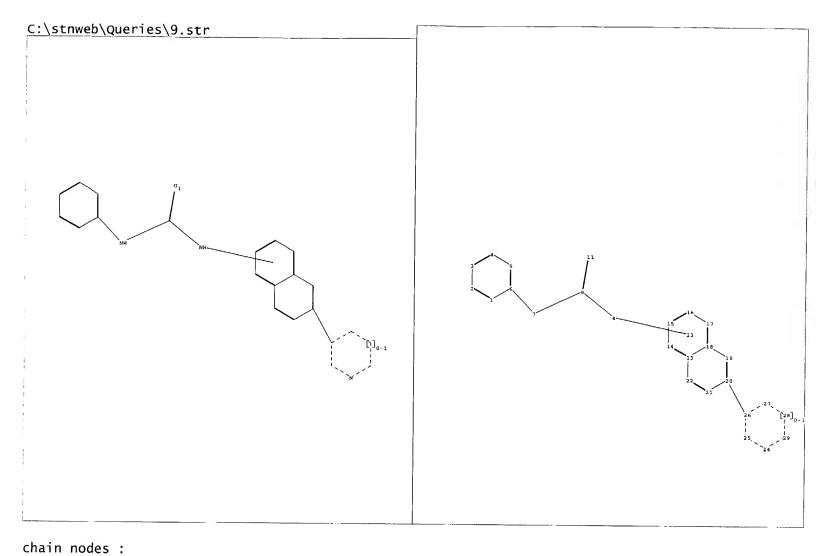
CN Carbanilide, 4-cyclopentyl- (6CI) (CA INDEX NAME)



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1 2 3 4 5 6 13 14 15 16 17 18 19 20 21 22 24 25 26 27 28 29
chain bonds:
6-7 7-9 8-9 9-11
ring bonds:
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 13-22 14-15 15-16 16-17 17-18 18-19 19-20 20-21 21-22 24-25 24-29 25-26 26-27 27-28 28-29
exact/norm bonds:
6-7 7-9 8-9 9-11
normalized bonds:
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 13-22 14-15 15-16 16-17 17-18 18-19 19-20 20-21 21-22 24-25 24-29 25-26 26-27 27-28 28-29
isolated ring systems:
containing 1: 13: 24:
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G1:0,S

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 11:CLASS
13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom



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7 8 9 11
ring nodes:
    1 2 3 4 5 6 13 14 15 16 17 18 19 20 21 22 24 25 26 27 28 29
chain bonds:
    6-7 7-9 8-9 9-11 20-26
ring bonds:
    1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 13-22 14-15 15-16 16-17 17-18 18-19 19-20 20-21 21-22 24-25 24-29 25-26 26-27 27-28 28-29
exact/norm bonds:
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exact bonds:
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normalized bonds:
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isolated ring systems:
    containing 1: 13: 24:
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G1:0,S

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 11:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom

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COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

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STRUCTURE FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9 DICTIONARY FILE UPDATES: 23 JUN 2004 HIGHEST RN 698346-19-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

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L1 HAS NO ANSWERS

L1 STR

=> s 11

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100.0% PROCESSED 112 ITERATIONS 22 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

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PROJECTED ANSWERS: 159 TO 721

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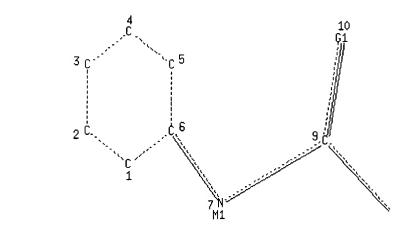
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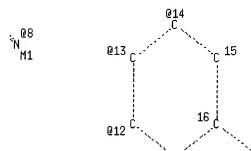
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L3 STR

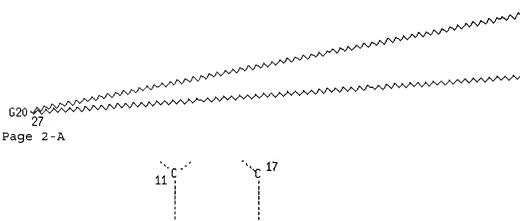
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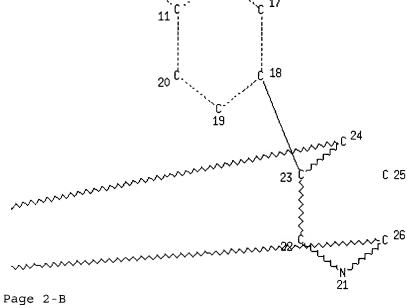


Page 1-A









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RSPEC I
NUMBER OF NODES IS 29
STEREO ATTRIBUTES: NONE
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SAMPLE SCREEN SEARCH COMPLETED - 18 TO ITERATE
100.0% PROCESSED
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                                                             0 ANSWERS
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                      BATCH **COMPLETE**
                       106 TO 614
PROJECTED ITERATIONS:
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             0 SEA SSS SAM L3
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FULL SCREEN SEARCH COMPLETED - 333 TO ITERATE
100.0% PROCESSED
                  333 ITERATIONS
                                                             0 ANSWERS
SEARCH TIME: 00.00.01
L5
            0 SEA SSS FUL L3
=> d his
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    FILE 'REGISTRY' ENTERED AT 20:56:55 ON 24 JUN 2004
L1
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L2
            22 S L1
              STRUCTURE UPLOADED
L3
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L4
L5
             0 S L4 FULL
=> s 12 full
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=> file hcaplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 317.98 318.19

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 16

L7 28 L6

=> s 17 and cirillo, p?/au 70 CIRILLO, P?/AU

L8 8 L7 AND CIRILLO, P?/AU

=> d 18, ibib abs fhitstr, 1-8

L8 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER: 2003:319714 HCAPLUS

DOCUMENT NUMBER: 138:338157

TITLE: Preparation of 1,4-disubstituted benzo-fused ureas as

cytokine inhibitors

INVENTOR(S): Cirillo, Pier F.; Hammach, Abdelhakim; Regan, John R.

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 100 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003032989	A1	20030424	WO 2002-US32809	20021011

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             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
             TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
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     US 2003162968
                       Α1
                            20030828
                                           US 2002-269173
                                                             20021011
PRIORITY APPLN. INFO.:
                                        US 2001-330254P P
                                                            20011018
OTHER SOURCE(S):
                         MARPAT 138:338157
GΙ
                    NV
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

The title compds. [I; ring A = fused (un)satd. ring contg. 3-5 carbon atoms (wherein ring A or the Ph ring to which it is fused is optionally substituted); G = (un)substituted 5-membered heteroaryl; Q = (un)substituted naphthyl, benzocyclobutanyl, indanyl, etc.; X = 0, S] which are active as anti-inflammatory agents, were prepd. Thus, reacting the carbamate II with the amine III (multi-step prepn. given) in DMSO afforded 84% urea IV. The preferred compds. I including those from the synthetic examples were evaluated for their inhibition of TNF α prodn. in THP cells, and showed IC50 < 10 μ M.

IT 515843-57-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 1,4-disubstituted benzo-fused ureas as cytokine inhibitors) 515843-57-9 HCAPLUS

RN 515843-57-9 HCAPLUS
CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[3-(2-pyridinylmethyl)-3H-imidazo[4,5-b]pyridin-6-yl]-1-naphthalenyl]- (9CI)
(CA INDEX NAME)

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

138:14065

Citing Full Text References

ACCESSION NUMBER:

2002:927403 HCAPLUS

DOCUMENT NUMBER:

TITLE:

Carbamate and oxamide compounds as inhibitors of

cytokine production

INVENTOR (S):

Cirillo, Pier F.; Kamhi, Victor; Regan, John

Robinson; Tsang, Michele

PATENT ASSIGNEE(S):

Boehringer Ingelheim Pharmaceuticals, Inc., USA;

Raymond, Robert, P.

SOURCE:

PCT Int. Appl., 109 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. -----WO 2002096876 A1 20021205 WO 2002-US14400 20020508 AE, AU, BG, BR, CA, CN, CO, CZ, EC, EE, HR, HU, ID, IL, IN, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR 20040310 EP 2002-731697 EP 1395561 Α1 20020508 AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR ÚS 2003092702 A1 20030515 US 2002-147675 20020517 US 6743788 B2 20040601 PRIORITY APPLN. INFO US 2001-293600P P 20010525 WO 2002-US14400 W 20020508 OTHER SOURCE(S): MARPAT 138:14065 GI

AB GEC(:W)NHArXYZ [G = (un)substituted heterocyclic; E = 0, NH, S; W = 0, S; Ar = (un) substituted Ph, naphthyl, indenyl, heterocyclic; X = (un) substituted cycloalkyl, cycloalkenyl, aryl, heterocyclic; Y = bond, (un) substituted alkylene, alkenylene, oxaalkylene, azaalkylene, thiaalkylene; Z = (un) substituted aryl, heteroaryl, NH2, OH, halogen, CN] were prepd. for treating cytokine mediated diseases or conditions such as chronic inflammatory diseases. Thus, 4-Me3CC6H4OMe was dinitrated, reduced to the monoamine, converted to the nitro isocyanate, treated with MeOCH2CH2OH, and reduced to 2-methoxyethoxy N-(3-amino-5-tert.-butyl-2methoxyphenyl)carbamate (I). 3-Bromoaniline was cyclized with (BrCH2CH2)20, converted to the tributylstannane, and coupled with 1-amino-4-bromonaphthalene to give 1-amino-4-(3morpholinophenyl)naphthalene which was N-protected with Cl3CCH2O2CCl and treated with I to give the carbamate II. Title compds. had IC50 for inhibition of TNF α < 10 μM .

IT 477699-48-2P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(carbamates and oxamides as inhibitors of cytokine prodn.)

477699-48-2 HCAPLUS

CN Carbamic acid, [5-(1,1-dimethylethyl)-2-methoxy-3-[[[[4-[6-(4morpholinylmethyl) -3-pyridinyl] -1-naphthalenyl] amino] carbonyl] amino] phenyl]-, 2-methoxyethyl ester (9CI) (CA INDEX NAME)

PAGE 2-A

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

4

Full Citing Text References

ACCESSION NUMBER: 2002:888719 HCAPLUS

DOCUMENT NUMBER: 137:384854

TITLE: Preparation of diaryl ureas as antiinflammatory agents

INVENTOR(S): Cirillo, Pier F.; Goldberg, Daniel R.; Hammach,

Abdelhakim; Moss, Neil; Regan, John Robinson

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA SOURCE:

PCT Int. Appl., 67 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

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PATENT NO.
                     KIND DATE
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    WO 2002092576
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                    A1
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                     Α1
                          20040303
                                         EP 2002-734324
                                                         20020508
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            IE, SI, LT, LV, FI, RO, CY, TR
    US 2003008868
                    A1 20030109
                                         US 2002-143322
                                                         20020510
PRIORITY APPLN. INFO.:
                                      US 2001-291425P P 20010516
                                      WO 2002-US14733 W 20020508
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AB The title diaryl ureas, useful in pharmaceutic compns. for treating a cytokine mediated diseases or conditions involving inflammation such as chronic inflammatory diseases, were prepd. Thus, treating 4-(2-chloropyrimidin-4-yloxy)naphthalen-1-ylamine with Et3N in DMF followed by addn. of Et4NCN, and treatment of the resulting nitrile with phosgene, and reacting the intermediate with 5-tert-butyl-o-anisidine afforded the urea I.

IT 473271-86-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of diaryl ureas as antiinflammatory agents)

Ι

RN <u>473271-86-2</u> HCAPLUS

CN Methanesulfonamide, N-[5-(1,1-dimethylethyl)-2-methoxy-3-[[[[4-[[2-[(2-pyridinylmethyl)amino]-4-pyrimidinyl]oxy]-1-naphthalenyl]amino]carbonyl]amino]phenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

Citing References Text

ACCESSION NUMBER: 2002:814102 HCAPLUS

DOCUMENT NUMBER:

TITLE:

Preparation of morpholine-containing aromatic and

heteroaromatic ureas as inhibitors of inflammatory

cytokines useful as anti-inflammatory agents

INVENTOR (S):

PATENT ASSIGNEE(S):

SOURCE:

Breitfelder, Steffen; Cirillo, Pier F.; Regan, John R. Boehringer Ingelheim Pharmaceuticals, Inc., USA

PCT Int. Appl., 120 pp.

CODEN: PIXXD2

137:325421

DOCUMENT TYPE:

Patent English

LANGUAGE:

FAMILY ACC. NUM. COUNT:

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		AZ,	BY,	KG,	KZ,	MD,	RƯ,	TJ,	TM								
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PRIORI	TY APP	LN.	INFO	. :				1	WO 20	001-T	JS12	253	W	2001	0413		
OTHER	SOURCE	(S):			CAS	REAC'	T 13'	7:32	5421	; MAI	RPAT	137	:325	421			
GI																	

AB Disclosed are novel arom. compds. (G-E-C(:W)-NH-Ar-X-Y-Z; e.g.1-[5-tert-butyl-3-(2-dimethylamino-3,4-dioxocyclobut-1-enylamino)-2methoxyphenyl]-3-[4-(6-morpholin-4-ylmethylpyridin-3-yl)naphthalen-1yl]urea (shown as I)) wherein G, E, W, Ar, X, Y and Z are defined in the claims. The compds. are useful for treating diseases or pathol. conditions involving inflammation, such as chronic inflammatory diseases. Also disclosed are pharmaceutical compns. contg. and processes of making such compds. Tests of preferred claimed compds. for inhibition of tumor necrosis factor (TNFa) prodn. in lipopolysaccharide stimulated THP cells showed IC50 < 10 µM. Sixteen example prepns, of intermediates and claimed compds. are provided. For example, to prep. I, 5-tert-butyl-2-methoxy-1,3-dinitrobenzene was added to EtOH under N2 purge and to this mixt., ammonium formate was added, followed by 10% Pd on C. To a soln. of the formed diamine in anhyd. MeOH at 0-5° was added 3,4-dimethoxycyclobutene-1,2-dione. To a soln. of the formed intermediate in THF at 0-5° was added dimethylamine in THF. To a mixt. of this intermediate in CH2Cl2 and satd. aq. NaHCO3 at 0-5° was added phosgene in toluene followed by 1-amino-4-(6-morpholin-4-ylmethylpyridin-3yl) naphthalene in anhyd. THF to give I. IT 294850-71-8P, N-Methanesulfonyl-N-[5-tert-Butyl-2-methoxy-3-[3-[4-(6-[(morpholin-4-yl)methyl]pyridin-3-yl)naphthalen-1yl]ureido]phenyl]methanesulfonamide RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

Ι

(Uses)

(drug candidate; prepn. of morpholine-contq. arom. and heteroarom. ureas as inhibitors of inflammatory cytokines useful as anti-inflammatory agents)

RN 294850-71-8 HCAPLUS

CN

Methanesulfonamide, N-[5-(1,1-dimethylethyl)-2-methoxy-3-[[[4-[6-(4-methylethyl)-2-methoxy-3-[]]]]morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]amino]carbonyl]amino]phenyl]-N-(methylsulfonyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN L8

3

Citing Full References Text ACCESSION NUMBER:

2002:814091 HCAPLUS

DOCUMENT NUMBER:

137:310705

TITLE:

Preparation of 1,4-disubstituted benzo-fused arylureas

for chronic inflammatory diseases

INVENTOR(S):

Cirillo, Pier F.; Goldberg, Daniel R.; Hammach,

Abdelhakim; Moss, Neil; Mueller, Kristen; Regan, John

Robinson

PATENT ASSIGNEE(S):

Boehringer Ingelheim Pharmaceuticals, Inc., USA

SOURCE:

PCT Int. Appl., 155 pp.

CODEN: PIXXD2 Patent

DOCUMENT TYPE: LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE ______ _ - - - - - -______ 20021024 WO 2002-US8504 20020321 WO 2002083628 Al

W: AE, AU, BG, BR, BY, CA, CN, CO, CZ, EC, EE, HR, HU, ID, IL, IN, JP, KR, KZ, LT, LV, MX, NO, NZ, PL, RO, RU, SG, SI, SK, UA, UZ,

VN, YU, ZA RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR EP 1381592 A1 20040121 EP 2002-723527 20020321 AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR US 2003083333 A1 20030501 US 2002-120028 20020410 PRIORITY APPLN. INFO.: US 2001-283642P P 20010413 WO 2002-US8504 W 20020321 OTHER SOURCE(S): CASREACT 137:310705; MARPAT 137:310705 GI

- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- AB Title compds. I [A = fused (un)satd. (un)substituted ring contg. 3-5 C atoms; G = Ph, naphthyl, benzocyclobutanyl, dihydronaphthyl, etc.; L = O, NH, CO, CS, etc.; Q = Ph, naphthyl, pyridinyl, pyrimidinyl, etc.; Y (covalently attached to Q) = O, CO, NH, CONH, etc.; n = 0-2; X = O, S] were prepd. For instance, 4-amino-1-naphthol•HCl was converted to the N-Boc deriv. and alkylated with 4-(2-chloroethyl)morpholine•HCl (CH3CN, K2CO3, 80°, 3 h); the product was deprotected to give 4-[2-(morpholin-4-yl)ethoxy]naphth-1-ylamine. This intermediate was reacted with phosgene (CH2Cl2/H2O/NaHCO3, 0°) and the resulting intermediate coupled to 5-tert-butyl-3-methylcarbamoyl-2-methoxyaniline (prepn. given) to afford II. I are useful in pharmaceutic compns. for treating, e.g., rheumatoid arthritis, osteoarthritis, Crohn's disease, etc.

IT 473269-78-2P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. of 1,4-disubstituted benzo-fused arylureas for chronic inflammatory diseases)

RN 473269-78-2 HCAPLUS

CN 2-Pyridinecarboxylic acid, 4-[[4-[[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]amino]-1-naphthalenyl]oxy]-, methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

MeO - C N

REFERENCE COUNT:

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

1

Full Citing Text References

ACCESSION NUMBER: 2002:185696 HCAPLUS

DOCUMENT NUMBER: 136:247592

TITLE: Preparation of heterocyclyl arylamides and ureas as

antiinflammatory agents

INVENTOR(S): Breitfelder, Steffen; Cirillo, Pier F.; Regan, John R.

PATENT ASSIGNEE(S): Germany

SOURCE: U.S. Pat. Appl. Publ., 36 pp., Cont.-in-part of U.S.

Ser. No. 505,582.

CODEN: USXXCO

Patent

DOCUMENT TYPE:

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION: NO PAGE 1

PATE	INT INFORMATION:	W /V 6	Word		
O	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ૣૻૺૼૼૼૼ	- US 2002032195	A1	20020314	US 2001-834797	20010413
60	US 6608052	B2	20030819		_
2	US 6358945 /	B1	20020319	US 2000-505582	20000216
100	US 2002055507 /	A1	20020509	US 2001-962709	20010925
	US 6660732)B2	20031209	HQ 2001 0620F7	20010025
-0	US 2002082256-	-γ A1	20020627 20031202	<u>US 2001-962057</u>	20010925
6-	<u>-US 6656933</u>	B2	20031202		

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US 2003065034
                                                     20030403
                                                                                 US 2002-264689
                                                                                                                 20021004
          US 6703525 - 16
                                           B2
                                                     20040309
          US 2003225077-10 A1
                                                     20031204
                                                                                 US 2003-424613
                                                                                                                 20030428
          US 2004019038 - A1
                                                     20040129
                                                                                 US 2003-624289
                                                                                                                 20030721
 PRIORITY APPLN. INFO.: (\(\))
                                                                           US 2000-505582 A2 20000216
                                                                           US 1999-124148P P 19990312
                                                                           <u>US 1999-165867P</u> P 19991116
                                                                           US 2001-834797 A2 20010413
                                                                           US 2001-962057 A1 20010925
                                                                           US 2001-962709
                                                                                                        A3 20010925
OTHER SOURCE(S):
                                               MARPAT 136:247592
         GEC(:W) NHArXYZ [E = O, NH, S; G = (substituted) Ph, naphthyl,
          benzocyclobutyl, dihydronaphthyl, benzocycloheptyl, indanyl, indenyl,
          pyridyl, quinolinyl, oxetanyl, pyrrolidinyl, piperidinyl, etc.; Ar =
          (substituted) Ph, naphthyl, quinolinyl, isoquinolinyl, tetrahydronaphthyl,
          benzofuryl, benzothienyl, benzimidazolyl, indanyl, etc.; X = (substituted)
          cycloalkyl, cycloalkenyl, aryl, furyl, thienyl, pyrrolyl, pyrazolyl,
          imidazolyl, pyridinyl, etc.; Y = bond, (substituted) (0-, S-, S0-, S02-,
          N-interrupted) alkylene; Z = (substituted) pyridinyl, piperazinyl,
         pyrimidinyl, pyrazinyl, imidazolyl, pyrazolyl, triazolyl, tetrazolyl,
          furyl, thienyl, etc.; W = 0, S], were prepd. Thus, 5-tert-butyl-2-methoxy-
          1,3-dinitrobenzene (prepn. given) was stirred with ammonium formate and
          Pd/C in EtOH followed by 3 h reflux to give 90% diamine, which in MeOH was
          treated with 3,4-dimethoxycyclobutene-1,2-dione at 0-5° followed by
         stirring and warming to room temp. to give an intermediate. The
          intermediate in THF was treated with Me2NH at 0-5° followed by
         stirring and warming to room temp. to give the dimethylamino intermediate.
         The latter in CH2Cl2 was treated with COCl2 in PhMe and aq. NaHCO3
         followed by removal of most volatiles. The residue was added to
         1-amino-4-(6-morpholin-4-ylmethylpyridin-3-yl)naphthalene (prepn. given)
         in THF followed by stirring overnight to give 1-[5-tert-butyl-3-(2-
         dimethylamino-3,4-dioxocyclobut-1-enylamino)-2-methoxyphenyl]-3-[4-(6-
         morpholin-4-ylmethylpyridin-3-yl)naphthalen-1-yl]urea. Preferred title
         compds. inhibited TNF \alpha prodn. in THP cells with IC50<10 \mu M.
IT 294850-71-8P
         RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
         (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
               (prepn. of heterocyclyl arylamides and ureas as antiinflammatory
               agents)
         294850-71-8 HCAPLUS
RN
         \label{lem:methode} \mbox{Methanesulfonamide, N-[5-(1,1-dimethylethyl)-2-methoxy-3-[[[4-[6-(4-1)]]]] and the lemma of the second control of the second c
CN
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CN Methanesulfonamide, N-[5-(1,1-dimethylethyl)-2-methoxy-3-[[[[4-[6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]amino]carbonyl]amino]phenyl]-N-(methylsulfonyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

HCAPLUS COPYRIGHT 2004 ACS on STN L8ANSWER 7 OF 8

Citing Full References ACCESSION NUMBER:

2001:380570 HCAPLUS

DOCUMENT NUMBER:

135:5453

TITLE:

Preparation of aromatic heterocyclic substituted urea derivatives as non-steroidal anti-inflammatory agents

INVENTOR(S):

Breitfelder, Steffen; Cirillo, Pier F.; Hao, Ming-Hong; Hickey, Eugene R.; Sharma, Rajiv; Sun,

Sanxing; Takahashi, Hidenori

PATENT ASSIGNEE(S):

Boehringer Ingelheim Pharmaceuticals, Inc., USA

SOURCE:

PCT Int. Appl., 88 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT NO.	KIND DATE	APPLICATION NO. DATE
WO 2001036403	Al 20010525	WO 2000-US31582 20001116
W: AE, AU,	BG, BR, BY, CA,	, CN, CZ, EE, HR, HU, ID, IL, IN, JP, KR,
KZ, LT,	LV, MX, NO, NZ,	, PL, RO, RU, SG, SI, SK, TR, UA, US, UZ,
VN, YU,		
RW: AT, BE,	CH, CY, DE, DK,	, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,

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PT, SE, TR
     EP 1232150
                       A1
                            20020821
                                           EP 2000-978751
                                                            20001116
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, ŞI, LT, LV, FI, RO, CY, TR
    US 6492393 🗸 🚧
                                           US 2000-714539
                       В1
                            20021210
                                                            20001116
     JP 2003514808
                       T2
                                           JP 2001-538892
                            20030422
                                                             20001116
     US 2003125354
                       Αl
                            20030703
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                                                             20021015
PRIORITY APPLN. INFO
                                        US 1999-165903P P
                                                            19991116
                                        US 2000-714539
                                                         A3 20001116
                                        WO 2000-US31582 W 20001116
OTHER SOURCE(S):
                         MARPAT 135:5453
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$$\begin{array}{c|c} & & & & & & & & & & & & & & & & \\ & & & & & & & & & & & & & & \\ & & & & & & & & & & & & \\ & & & & & & & & & & & \\ & & & & & & & & & & \\ & & & & & & & & & & \\ & & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & \\ & & \\ \\ & \\ & \\ \\ & \\ & \\ \\ & \\ & \\ \\ & \\ & \\ \\ & \\ \\ & \\ \\ & \\ \\ & \\ \\ & \\ \\ & \\ \\ & \\$$

Title compds. (I) [wherein G = (un)substituted (non)arom. carbocycle or heterocycle; Ar = (un)substituted Ph, (tetrahydro)naphthyl, (tetrahydro)quinolinyl, (tetrahydro)isoquinolinyl, (dihydro)benzofuranyl, dihydrobenzothienyl, indolenyl, benzothiophenyl, benzimidazolyl, indanyl, indenyl, or indolyl; L = (un)substituted (un)satd. C chain with one or more methylene groups optionally independently replaced by O, N, or S(O)m; Q = (un)substituted Ph, naphthyl, pyridinyl, pyrimidinyl, pyridazinyl, (benz)imidazolyl, furanyl, thenyl, pyranyl, etc.; m = 0-2; X = O or S] were prepd. as cytokine prodn. inhibitors for use as non-steroidal anti-inflammatory agents. Thus, 4-[2-(morpholin-4-yl)ethoxy]naphth-1-ylamine was treated sequentially with phosgene and 5-tert-butyl-2-methylaniline in CH2Cl2 to give II (42%). In a cytokine prodn. inhibition assay, II inhibited TNFα in lipopolysaccharide stimulated THP cells with IC50 < 10 μM.</p>

IT 340825-40-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of arom. heterocyclic substituted urea derivs. as cytokine inhibitors for use as non-steroidal anti-inflammatory agents)

RN 340825-40-3 HCAPLUS

CN Urea, N-[4-[(2-amino-4-pyridinyl)oxy]-1-naphthalenyl]-N'-[5-(1,1-dimethylethyl)-2-methylphenyl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER: DOCUMENT NUMBER:

TITLE:

2000:666713 HCAPLUS

133:252426

Preparation of aromatic heterocyclic ureas as

antiinflammatory agents

INVENTOR(S): Betag

Betageri, Rajashehar; Breitfelder, Steffen; Cirillo, Pier F.; Gilmore, Thomas A.; Hickey, Eugene R.; Kirrane, Thomas M.; Moriak, Monica H.; Moss, Neil; Patel, Usha R.; Proudfoot, John R.; Regan, John R.; Sharma, Rajiv; Sun, Sanxing; Swinamer, Alan D.;

Talashanki Wilamani

Takahashi, Hidenori

PATENT ASSIGNEE(S):

SOURCE:

LANGUAGE:

Boehringer Ingelheim Pharmaceuticals, Inc., USA

PCT Int. Appl., 282 pp.

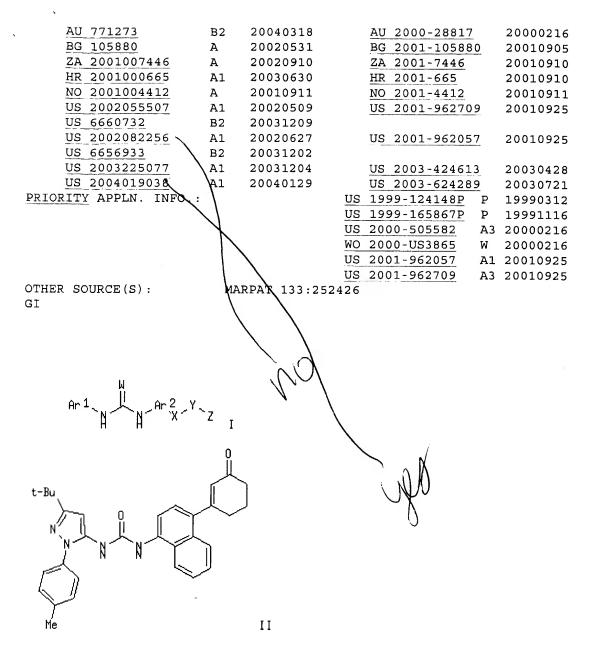
CODEN: PIXXD2

DOCUMENT TYPE:

Patent English

FAMILY ACC. NUM. COUNT:

PATENT NO.	KIND DA	ATE	APPLICATION NO.	DATE
WO 2000055139	A2 20	0000921	WO 2000-US3865	20000216
WO 2000055139	A3 20	0010426		
W: AE, AU,	BG, BR, B	BY, CA, CN,	CZ, EE, HR, HU, ID,	IL, IN, JP, KR,
KZ, LT,	LV, MX, N	NO, NZ, PL,	RO, RU, SG, SI, SK,	TR, UA, UZ, VN,
YU, ZA				
RW: AT, BE,	CH, CY, D	DE, DK, ES,	FI, FR, GB, GR, IE,	IT, LU, MC, NL,
PT, SE				
EP 1165516	A2 20	0020102	EP 2000-907295	20000216
R: AT, BE,	CH, DE, D	OK, ES, FR,	GB, GR, IT, LI, LU,	NL, SE, MC, PT,
IE, SI,	LT, LV, F	FI, RO		
BR 2000008922			BR 2000-8922	20000216
TR 200102817	T2 20	0020521	TR 2001-200102817	20000216
JP 2002539198	T2 20	0021119	JP 2000-605569	20000216
EE 200100483	A 20	0021216	EE 2001-483	20000216
NZ 514711	A 20	0040227	NZ 2000-514711	20000216



AB The title compds. (I) [wherein Ar1 = (un) substituted pyrrole, pyrrolidine, pyrazole, imidazole, oxazole, thiazole, furan, or thiophene; Ar2 = (un) substituted Ph, (tetrahydro) naphthyl, (tetrahydro) quinoline, (tetrahydro)isoquinoline, benzimidazole, benzofuran, indanyl, indenyl, or indole; W = O or S; X = (un)substituted cycloalkyl, cycloalkenyl, Ph, furan, thiophene, pyrrole, imidazolyl, pyridine, pyrimidine, (dihydro)pyridinone, (dihydro)maleimide, piperidine, piperazine, or pyrazine; Y = a bond or (un) substituted satd. or unsatd. alkyl optionally interrupted by O, NH, S(O), SO2, or S; Z = (un)substituted <math>Ph, pyridine, pyrimidine, pyridazine, imidazole, (tetrahydro)furan, thiophene, (tetrahydro)pyran, 1,3-dioxolanone, 1,3-dioxanone, 1,4-dioxane, (thio)morpholine (sulfoxide), piperidine, cyclohexanone, pentamethylene sulfoxide, etc.] were prepd. for the treatment of diseases or pathol. conditions involving inflammation, such as chronic inflammatory diseases. Thus, coupling 2-cyclohexenone with 4-bromo-1-naphthylamine in the presence of Pd(PPh3)2Cl2, DPPP, and NaHCO3 in DMF, followed by conversion of the amine to an isocyanate using ClCOCl and immediate addn. of 1-(4-methylphenyl)-3-tert-butyl-1H-pyrazol-5-amine, gave the urea II. a cytokine prodn. inhibition assay, preferred compds. of the invention

showed IC50 < 10 μM against TNF- α in lipopolysaccharide stimulated THF cells.

IT 294849-72-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of arom. heterocyclic urea antiinflammatory agents by conversion of arylamines to isocyanates followed by addn. of heterocyclic amines)

RN 294849-72-2 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)phenyl]-N'-[4-[6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

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(FILE 'HOME' ENTERED AT 20:56:40 ON 24 JUN 2004)

FILE 'REGISTRY' ENTERED AT 20:56:55 ON 24 JUN 2004
L1 STRUCTURE UPLOADED
L2 22 S L1
L3 STRUCTURE UPLOADED
L4 0 S L3
L5 0 S L4 FULL
L6 377 S L2 FULL

FILE 'HCAPLUS' ENTERED AT 21:08:09 ON 24 JUN 2004 28 S L6

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             20 L7 NOT L8
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            151 PATEL, U?/AU
 L10
              0 L9 AND PATEL, U?/AU
 => s 19 and proudfoot, j?/au
            249 PROUDFOOT, J?/AU
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 => s 19 and swinamer, a?/au
              9 SWINAMER, A?/AU
 L12
              0 L9 AND SWINAMER, A?/AU
 => s 19 and takahashi, h?/au
          12788 TAKAHASHI, H?/AU
 T.13
              0 L9 AND TAKAHASHI, H?/AU
 => s 19 and gilmore, t?/au
            151 GILMORE, T?/AU
 L14
              0 L9 AND GILMORE, T?/AU
 => s 19 and sharma, r?/au
           5153 SHARMA, R?/AU
              0 L9 AND SHARMA, R?/AU
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      ANSWER 1 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
            Citing
    Full
    Text
          References
                          2004:433797 HCAPLUS
 ACCESSION NUMBER:
 DOCUMENT NUMBER:
                          140:423477
 TITLE:
                          Preparation of diaryl ureas as inhibitors of p38
                          kinase
 INVENTOR (S):
                         Miller, Scott; Osterhout, Martin; Dumas, Jacques;
                          Khire, Uday; Lowinger, Timothy B.; Scott, William J.;
                         Smith, Roger A.; Wood, Jill E.; Gunn, David E.;
                         Hatoum-Mokdad, Holia; Rodriguez, Marell; Sibley,
                          Robert; Wang, Ming; Turner, Tiffany; Brennan,
                          Catherine
 PATENT ASSIGNEE(S):
                         Bayer Corporation, USA
 SOURCE:
                         U.S. Pat. Appl. Publ., 60 pp., Cont. of U.S. Ser. No.
                         458,015, abandoned.
                         CODEN: USXXCO
DOCUMENT TYPE:
                         Patent
LANGUAGE:
                         English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:
     PATENT NO.
                     KIND DATE
                                          APPLICATION NO. DATE
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                      _ - - -
                                           ______
     US 2004102636
                     A1
                            20040527
                                           US 2002-60396
                                                            20020201
PRIORITY APPLN. INFO.:
                                        US 1997-126439P P 19971222
                                        US 1998-285522 B1 19981222
                                        US 1999-458015 B1 19991210
AB
     A method of treating a p-38 mediated disease other than cancer comprises
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administration of BNHCONHA [A = (substituted) Ph, pyridyl, 2-thienyl; B = (substituted) aryl, heteroaryl contg. ≥ 1 6-membered arom. structure contg. 0-4 N, O, or S atoms]. Thus, 5-tert-butyl-2-(3-tetrahydrofuranyloxy)aniline (prepn. given) and p-tolyl isocyanate were stirred 8 h in PhMe to give 75% N-(5-tert-butyl-2-(3-tetrahydrofuranyloxy)phenyl)-N'-(4-methylphenyl)urea. Title compds. inhibited p38 kinase with IC50 = 1-10 μ M.

IT 228400-63-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of diaryl ureas as inhibitors of p38 kinase)

RN 228400-63-3 HCAPLUS

CN Urea, N-(3-methoxy-2-naphthalenyl)-N'-[4-(4-pyridinylthio)phenyl]- (9CI) (CA INDEX NAME)

L9 ANSWER 2 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER: 2004:142968 HCAPLUS

DOCUMENT NUMBER: 140:193056

TITLE: Combinations of active agents with p38 MAP kinase

inhibitors, pharmaceutical compositions, and use in

the treatment of cytokine-mediated diseases

INVENTOR(S): Simianer, Stefan; Bilbault, Pascal; Cappola, Michael

L.; Way, Susan Lynn

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA;

Boehringer Ingelheim France

SOURCE: PCT Int. Appl., 168 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PAT	CENT :	NO.		KI	ND	DATE			A.	PPLI	CATI	ON N	ο.	DATE			
WO	2004	0143	87	A	1	2004	0219		W	20	03-U	5253	41	2003	0812		
-	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	ΚP,	KR,	KZ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	OM,
		PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	ΤJ,	TM,	TN,
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		CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,
		NL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,
		GW,	ML,	MR,	NE,	SN,	TD,	TG									
US	2004	1107	55	A.	1 .	2004	0610		<u>U</u> :	5 20	03-6	3870:	2	2003	0811		
PRIORITY	APP:	LN.	INFO	. :				Ţ	US 20	002-	4031	15P	P	2002	0813		

GΙ

AB The invention relates to pharmaceutical combination therapies based on p38 kinase inhibitors and another active ingredients, pharmaceutical compns. comprising such combinations, processes for prepg. them, and their use in the treatment of cytokine-mediated diseases. Prepn. of I (BIRB 796 BS) is described.

I

IT 294849-84-6

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (combinations of active agents with p38 MAP kinase inhibitors, pharmaceutical compns., and use in treatment of cytokine-mediated diseases)

RN 294849-84-6 HCAPLUS

CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

REFERENCE COUNT:

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

7

Citing Full References

ACCESSION NUMBER:

2004:142601 HCAPLUS

DOCUMENT NUMBER:

140:193063

TITLE:

Anticoagulant and fibrinolytic therapy using p38 MAP

kinase inhibitors

INVENTOR(S):

Wood, Chester C.; Van Der Poll, Tom

PATENT ASSIGNEE(S):

Boehringer Ingelheim Pharmaceuticals, Inc., Germany;

APPLICATION NO. DATE

Boehringer Ingelheim Pharma GmbH & Co. KG

SOURCE:

U.S. Pat. Appl. Publ., 47 pp.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

KIND DATE

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.

	US	2004	0332	22	A	1 :	2004	0219		U	S 20	03-6	3059	9 :	2003	0730		
	WO	2004	0162	67	Α	1 :	2004	0226		W	0 20	03 - U	S238	41 :	2003	0730		
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
			CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
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PAGE 1-A

PAGE 2-A

ANSWER 4 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

Citing Full Text References ACCESSION NUMBER:

2004:41274 HCAPLUS

DOCUMENT NUMBER: 140:99644

TITLE: Pharmaceutical compositions based on novel anticholinergics and p38 kinase inhibitors

INVENTOR(S): Pairet, Michel; Meade, Christopher John Montague;

Pieper, Michael P.

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma G.m.b.H. & Co. K.-G.,

Germany

Patent

SOURCE: PCT Int. Appl., 190 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

English

LANGUAGE:

FAMILY ACC. NUM. COUNT:

PAT	ENT	NO.		KI	ND	DATE			Α	PPLI	CATI	ON N	ο.	DATE			
		-		- -					-					- 	- 		
WO	2004	0047	25	A	2	2004	0115		W	0 20	03-E	P673	9	2003	0626		
WO	2004	0047	25	A	3	2004	0527										
	W:	AE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
		co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	ΚP,	KR,	KZ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	OM,
		PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	ТJ,	TM,	TN,	TR,
		TT,	TZ,	UA,	ŪĠ,	US,	UΖ,	VC,	VN,	YU,	ZA,	ZM,	ZW,	AM,	AZ,	BY,	KG,
		KZ.	MD.	RU.	TJ												

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

<u>US 2004044020</u> A1 20040304

US 2003-611717 20030701 EP 2002-15231 A 20020709

PRIORITY APPLN. INFO.:

US 2002-407733P P 20020903

OTHER SOURCE(S):

MARPAT 140:99644

GΙ

- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- AB The present invention relates to novel pharmaceutical compns. based on novel anticholinergics and p38 kinase inhibitors, processes for prepg. them and their use in the treatment of respiratory diseases. Inhalation powders were prepd. contg. anticholinergic I and p38 kinase inhibitor II.

IT 294849-84-6

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (pharmaceutical compns. based on novel anticholinergics and p38 kinase inhibitors)

RN 294849-84-6 HCAPLUS

CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

L9 ANSWER 5 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

Citing

ACCESSION NUMBER:

2003:818257 HCAPLUS

DOCUMENT NUMBER:

139:312451

TITLE:

Inhalant p38 kinase inhibitor formulations for

treating mucus hypersecretion

INVENTOR(S):

Jung, Birgit

PATENT ASSIGNEE(S):

Boehringer Ingelheim Pharma G.m.b.H. & Co. K.-G.,

Germany

SOURCE:

PCT Int. Appl., 191 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

P.	ATENT	NO.		KI	ND	DATE			A:	PPLI	CATI	и ис	٥.	DATE			
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WC	2003	0845	03	A.	2	2003	1016		W	20	03-E	P343	4	2003	0402		
WC	2003	0845	03	A.	3	2004	0408										
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		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
		GM,	HR,	HU,	ID,	ΙL,	IN,	IS,	JP,	KE,	KG,	ΚP,	KR,	KZ,	LC,	LK,	LR,
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		GW,	ML,	MR,	NE,	SN,	TD,	TG									
US	2003	2203	36	A:	1	2003	1127		US	3 200	3-40	0042	1	2003	0327		
PRIORIT	Y APP	LN.	INFO	. :				3	EP 20	002-1	7699		A	20020	0405		
								1	JS 20	002-3	858	56P	P	20020	0605		
OTHER S	OURCE	(S):			MAR	PAT :	139:3	3124	5 1								

GΙ

AΒ The invention relates to the use of p38 kinase inhibitors for the prepn. of a pharmaceutical compn. suitable for inhalation for the treatment of mucus hypersecretion. Furthermore the invention is directed to pharmaceutical compns. suitable for inhalation comprising p38 kinase inhibitors such as I and methods for their prepn.

Ι

IT 294849-84-6

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (inhalant p38 kinase inhibitor formulations for treating mucus hypersecretion)

. RN 294849-84-6 HCAPLUS

CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

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L9 ANSWER 6 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing
Text References
ACCESSION NUMBER:

2003:656575 HCAPLUS

DOCUMENT NUMBER: 139:197476

TITLE: Preparation of aryl heterocyclyl ureas with raf kinase

and angiogenesis inhibiting activity

INVENTOR(S): Dumas, Jacques; Scott, William J.; Elting, James;

Hatoum-Makdad, Holia
NEE(S): Bayer Corporation, USA

PATENT ASSIGNEE(S): Bayer Corporation, USA SOURCE: PCT Int. Appl., 142 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT N	10.		KI	ND :	DATE			A)	PPLI	CATIO	ON NO	o. :	DATE			
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WO 20030	6822	3	A:	1	2003	0821		W	20	03-U	S410:	2	2003	0211		
W:	AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	ΚP,	KR,	KΖ,	LC,	LK,	LR,
	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,

PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 2004023961 A1 20040205 US 2003-361844 20030211

PRIORITY APPLN. INFO.: US 2002-354948P P 20020211

AB 283 Of the title ureas useful for treating diseases mediated by raf kinase and diseases mediated by the VEGF induced signal transduction pathway characterized by abnormal angiogenesis or hyperpermeability processes, were claimed. Synthesis of 6 ureas such as I was described. Thus, reacting 3-(tert-butyl)-1-(4-methylphenyl)pyrazole-5-ylamine with 4-(2-morpholin-4-ylethoxy)naphthylamine (prepns. given) and CDI in CH2Cl2 afforded 80% I which showed IC50 of < 1 µM in in vitro raf kinase and in in vitro Flk-1 ELISA assay.

I

IT 294849-72-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of aryl heterocyclyl ureas with raf kinase and angiogenesis inhibiting activity)

RN 294849-72-2 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)phenyl]-N'-[4-[6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

t-Bu

REFERENCE COUNT:

17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 7 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER:

2003:221509 HCAPLUS

DOCUMENT NUMBER:

138:231790

TITLE:

Methods using aromatic heterocyclyl compounds for

treating cytokine-mediated diseases

INVENTOR(S):

Moss, Neil; Regan, John R.

PATENT ASSIGNEE(S):

Boehringer Ingelheim Pharmaceuticals, Inc., USA

PCT Int. Appl., 175 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

SOURCE:

English

FAMILY ACC. NUM. COUNT:

P	ATENT	NO.		KI	ND I	DATE			A	PPLI	CATI	ON NO	o. :	DATE				
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W	0 2003	0222	73	A	1 :	2003	0320		W	20	02-U	S286	<u> 15</u>	2002	909			
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		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,	
		PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TN,	TR,	TT,	TZ,	
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	RW:	GH,	GM,	ΚE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AT,	BE,	BG,	
		CH.	CY.	CZ.	DE.	DK.	EE.	ES.	FI.	FR.	GB.	GR.	TE.	TT.	T _i U.	MC.	NL.	

PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,

NE, SN, TD, TG

20030327 Α1 **A1** 20040616 US 2002-237306 20020909

EP 2002-797884 20020909

AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK

PRIORITY APPLN. INFO.:

US 2003060455

EP 1427412

US 2001-318958P P 20010913 WO 2002-US28615 W 20020909

OTHER SOURCE(S):

MARPAT 138:231790

Methods are disclosed for treating acute and chronic inflammation in the lung caused by inhalation of smoke, endometriosis, Behcet's disease, uveitis, ankylosing spondylitis, pancreatitis, cancer, Lyme disease, sepsis, chronic obstructive pulmonary disease, traumatic arthritis, congestive heart failure and restenosis percutaneous transluminal coronary angioplasty, known to be cytokine mediated, using arom. heterocyclic compds. described in WO 00/55139.

IT 294850-09-2

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(arom. heterocyclyl compds. for treating cytokine-mediated diseases)

RN 294850-09-2 HCAPLUS

Urea, N-[3-(2,3-dihydroxypropyl)-5-(1,1-dimethylethyl)-2-hydroxyphenyl]-N'-CN[4-[6-(4-morpholinylmethyl)-3-pyridinyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT L9 ANSWER 8 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER: 2000:98559 HCAPLUS

DOCUMENT NUMBER: 132:137410

TITLE: Preparation of novel azabicyclic compounds for

treatment of CNS disorders

INVENTOR(S): Gaster, Laramie Mary; Heightman, Thomas Daniel; Wyman,

Paul Adrian

PATENT ASSIGNEE(S): Smithkline Beecham PLC, UK SOURCE: PCT Int. Appl., 40 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

WO 2000006575 A2 20000210 WO 1999-EP5350 19990723

WO 2000006575 A3 20000518

W: CA, JP, US

RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,

PT, SE

<u>PRIORITY</u> APPLN. INFO.: <u>GB 1998-16288</u> A 19980728

GB 1998-27881 A 19981217

OTHER SOURCE(S): MARPAT 132:137410

GΙ

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

The title compds. [I; Ra = II-IV (wherein P1-P3 = Ph, bicyclic aryl, 5-7 membered heterocyclyl, etc.; R1 = H, halo, alkyl, etc.; R2-R3 = halo, alkyl, cycloalkyl, etc.; a, b = 0-2; A = a bond, O, CH2, etc.; E = (un)substituted 5-7 membered carbocyclic ring fused at the 2,3- or 3,4-positions of the adjacent Ph ring, the ring E optionally fused to a further (un)substituted Ph ring); L = C(:V)DG, DGC(:V), YC(:V)DG; V = O, S; Y = NH, N(alkyl), CH2, O; D = N, C, CH; G = H, alkyl; Rb1, Rb2 = H, halo, OH, etc.; R4 = (un)substituted V (X = N, CH, C; m = 1-3), VI], useful in the treatment of CNS disorders such as depression, were prepd. Thus, treatment of 4-(pyridin-4-yl)naphth-1-ylamine with triphosgene in the presence of Et3N in DCM followed by addn. of (S)-4-methoxy-3- (octahydropyrrolo[1,2-a]pyrazin-2-yl)aniline in DCM afforded 91% (S)-VII. All presented examples of compds. I had pKi > 7.4 at 5-HT1A, 5-HT1B and 5-HT1D receptors.

IT 256923-80-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of novel azabicyclic compds. for treatment of CNS disorders)

RN <u>256923-80-5</u> HCAPLUS

CN Urea, N-[3-[(8aS)-hexahydropyrrolo[1,2-a]pyrazin-2(1H)-yl]-4-methoxyphenyl]-N'-[4-(4-pyridinyl)-1-naphthalenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L9 ANSWER 9 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing
Text References
ACCESSION NUMBER:

ACCESSION NUMBER: DOCUMENT NUMBER:

TITLE:

1999:421667 HCAPLUS

131:58659

Preparation of diaryl ureas as inhibitors of p38

kinase.

INVENTOR(S):

Miller, Scott; Osterhout, Martin; Dumas, Jacques; Khire, Uday; Lowinger, Timothy Bruno; Riedl, Bernd; Scott, William J.; Smith, Roger A.; Wood, Jill E.; Gunn, David; Hatoum-Mokdad, Holia; Rodriguez, Mareli;

Sibley, Robert; Wang, Ming

PATENT ASSIGNEE(S):

SOURCE:

Bayer Corporation, USA PCT Int. Appl., 107 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PA	TENT	NO.		KI	ND	DATE			A	PPLI	CATI	ои ис	٥.	DATE				
	WO	9932	463		A	 1	1999	0701		W	0 19	98-U	5272	 65	1998	1222			
		W:													CN,		CZ,	DE.	
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	AU	9919	399		A:	1	1999	0712		Αī	J 19	99-19	399		1998	1222			
	EP	1042	305		A:	1	2000	1011		E	2 19	98-96	5422	l	1998	1222			
		R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	
			ΙE,	SI,	LT,	LV,	FI,	RO											
	JP	2001	5262	76	T:	2	2001	1218		J	200	00-52	25400)	1998	1222			
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OTHER SOURCE(S): MARPAT 131:58659

AB A method of treating a p-38 mediated disease other than cancer comprises administration of BNHCONHA [A = (substituted) Ph, pyridyl, 2-thienyl; B = (substituted) aryl, heteroaryl contg. ≥1 6-membered arom. structure contg. 0-4 N, O, or S atoms]. Thus, 5-tert-butyl-2-(3-

tetrahydrofuranyloxy)aniline (prepn. given) and p-tolyl isocyanate were stirred 8 h in PhMe to give 75% N-(5-tert-butyl-2-(3-tetrahydrofuranyloxy)phenyl)-N'-(4-methylphenyl)urea. Title compds. inhibited p38 kinase with IC50 = 1-10 μ M.

IT 228400-63-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of diaryl ureas as inhibitors of p38 kinase)

RN 228400-63-3 HCAPLUS

CN Urea, N-(3-methoxy-2-naphthalenyl)-N'-[4-(4-pyridinylthio)phenyl]- (9CI) (CA INDEX NAME)

5

REFERENCE COUNT:

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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 L7
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 L8
                20 S L7 NOT L8
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 L16
                2 L6
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 L16 ANSWER 1 OF 2 CAOLD COPYRIGHT 2004 ACS on STN
       CA59:13238e CAOLD
       hydrazides - (XVII) hydrazones and thioureas with antituberculous activity
 ΤI
       Budeanu, Constantin H.; Budeanu, E.; Gaiginschi, A.; Radu C.
 ΑU
 IT <u>52540-96-2</u> <u>88513-18-2</u> <u>92160-05-9</u> <u>92160-56-0</u> <u>93535-33-2</u> <u>94461-81-1</u>
       \underline{95942-51-1} \quad \underline{98396-42-0} \quad \underline{100027-18-7} \quad \underline{100150}-24-1 \quad \underline{100259}-97-0 \quad \underline{100265-63-2}
       100660-40-0 101015-77-4 101201-07-4
 L16 ANSWER 2 OF 2 CAOLD COPYRIGHT 2004 ACS on STN
     CA59:5124e CAOLD
 AN
       hydrazides - (XIV) derivs. of isonicotinoyl hydrazide, (XV) thiourea
 TI
       derived from the isonicotinoylhydrazone of p-aminoacetophenone
 ΑU
       Budeanu, Constantin H.
                    <u>4456-77-3</u> <u>26051-66-1</u> <u>52540-96-2</u> <u>91642-09-0</u> <u>92160-05-9</u>
 IT
       895-82-9
       92160-56-0 \quad \underline{92193-14-1} \quad \underline{93535-33-2} \quad 95942-51-1 \quad \underline{98396-42-0} \quad \underline{100027-18-7}
       100150-24-1 100259-97-0 100265-63-2 100660-40-0 101015-77-4 101201-07-4
 => fil reg; d acc 101201-07-4; fil CAOLD
 FILE 'REGISTRY' ENTERED AT 21:19:38 ON 24 JUN 2004
 ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN
       101201-07-4 REGISTRY
       Isonicotinic acid, [α-methyl-p-[3-(1-naphthyl)-2-
       thioureido]benzylidene]hydrazide (7CI) (CA INDEX NAME)
      3D CONCORD
 FS
 MF
      C25 H21 N5 O S
 SR
      CAOLD
     STN Files: CA, CAOLD, CAPLUS
 DT.CA CAplus document type: Journal
 RL.NP Roles from non-patents: NORL (No role in record)
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PAGE 1-A

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 2 REFERENCES IN FILE CA (1907 TO DATE)
- 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- 2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

FILE 'CAOLD' ENTERED AT 21:19:39 ON 24 JUN 2004

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